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ISENTROPIC FLOW SOLUTIONS FOR REACTING GAS MIXTURES IN THERMOCHEMICAL EQUILIBRIUM

by Ernest V. Zoby, Jane T. Kemper, and Casimir J. Jachimowski

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ISENTROPIC FLOW SOLUTIONS FOR REACTING GAS MIXTURES IN THERMOCHEMICAL EQUILIBRIUM

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SUMMARY

A machine program has been developed for the calculation of local (edge of the boundary layer) pressure, density, temperature, enthalpy, entropy, the mole fractions of the chemical species, velocity, and the derivative of the velocity with respect to the pressure over a blunt body from given free-stream conditions. The local values are computed for arbitrary reacting ideal gas mixtures in thermochemical equilibrium with the assumption of isentropic flow and a given pressure distribution over the body. Also, the associated normal shock and stagnation-point parameters are computed. Excellent correlations are obtained with existing solutions for air at free-stream velocities from 2000 to 50 000 ft/sec (0.6096 to 15.24 km/sec) and altitudes up to 300 000 ft (91.44 km). Also, results for the normal-shock, stagnation-point, and local conditions based on an assumed Martian atmosphere are presented. The program was developed for the IBM 7094 electronic computer at Langley Research Center. The identification of the program inputs, a flow diagram, a listing of the species and the program, and a sample input and output are given in the appendixes of the paper.

INTRODUCTION

For the calculation of local, blunt-body aerodynamic heat transfer and shear stress (for example, ref. 1), it is necessary to know the local (edge of the boundary layer) conditions over the blunt body. With known stagnation-point conditions, a given pressure distribution over the body, and the assumption of isentropic flow, the local conditions can be obtained from a Mollier diagram or by a curve-fit technique. However, these processes of obtaining the local conditions are time-consuming and usually result in a loss of accuracy.

Stagnation-point solutions with corresponding normal-shock data, Mollier diagrams, and curve fits to the Mollier diagram are available for an air model. (See refs. 2 to 7.) However, for gas models other than air (for example, Mars), these aids for computing the local conditions are not available.

Because of the problems of time consumption, inaccuracies, and insufficient sources of data, a computer program to calculate local conditions for blunt-body reentry in arbitrary gas mixtures is required. The only known programs which apply to the expansion of reacting gas mixtures are nozzle flow programs (for example, ref. 8). These programs require computed stagnation values and given area ratios and, consequently, are not readily adapted to a blunt-body reentry problem. Therefore, a program for the calculation of local, blunt-body conditions and the accompanying normal-shock and stagnation-point conditions from given free-stream conditions has been developed. The program combines the normal-shock relations and a general thermochemical equilibrium program for arbitrary ideal gas mixtures (ref. 9) with the assumption of isentropic flow and a known pressure distribution over the body. Since the equilibrium calculations of reference 9 are used, the blunt-body local conditions and the corresponding heating rates and shear stress values can now be computed for arbitrary reacting gas mixtures.

This paper describes the operation of the program, compares existing solutions for an air model with the present results, presents results based on an assumed Martian atmosphere, and includes program inputs (appendix A), flow diagrams (appendix B), listing (appendix C), and a sample input and output case (appendix D).

SYMBOLS

H	enthalpy, ergs/g
$\overline{M}$	molecular weight of mixture
p	pressure, dynes/cm^2
R	universal gas constant, ergs/mole-$^{\circ}$K
T	temperature, $^{\circ}$K
U	velocity, km/sec
x	distance from stagnation point corresponding to pressure, cm
x_i	mass fraction for species i
y_i	mole number for species i, moles of species i/gram of mixture
ρ	density, g/cc

S/R	entropy
ϵ	convergence criteria in stagnation point and local flow solution
τ	convergence criteria in normal-shock solution ($=10^{-5}$)

Subscripts:

a	denotes enthalpy change across shock based on equation (5)
b	denotes enthalpy change across shock based on equilibrium program
1	conditions ahead of shock
2	conditions behind shock
e	local flow conditions
s	stagnation-point conditions
i	denotes species
n	denotes iteration

METHOD OF CALCULATION

The one-dimensional steady flow of a gas through a normal-shock wave is given by the following equations:

$$\rho_1 U_1 = \rho_2 U_2 \tag{1}$$

$$p_1 + \rho_1 U_1^2 = p_2 + \rho_2 U_2^2 \tag{2}$$

$$H_1 + \frac{1}{2} U_1^2 = H_2 + \frac{1}{2} U_2^2 \tag{3}$$

These equations describe the requirements of mass, momentum, and energy conservation.

From these equations and the equation of state

$$p = \rho \frac{R}{\overline{M}} T \tag{4}$$

the following equations are obtained:

$$\Delta H_a = \frac{1}{2} U_1{}^2 \left[1 - \left(\frac{\rho_1}{\rho_2}\right)^2\right] \tag{5}$$

$$p_2 = p_1 \left\{1 + \frac{\overline{M}_1 U_1{}^2}{RT_1} \left[1 - \left(\frac{\rho_1}{\rho_2}\right)\right]\right\} \tag{6}$$

$$\frac{\rho_1}{\rho_2} = \frac{p_1 \overline{M}_1 T_2}{p_2 \overline{M}_2 T_1} \tag{7}$$

The equilibrium flow calculations are performed by using an equilibrium program developed by Allison (ref. 9), which utilizes the partition function of statistical thermodynamics to determine the thermodynamic parameters and a free-energy of minimization technique by White (ref. 10) to determine the equilibrium composition of the gas. Also, the necessary thermochemical data are listed in reference 9. The thermodynamic properties obtained with the general thermochemical equilibrium program for arbitrary ideal gas mixtures are compared with the results of other investigations in references 11 and 12. The program provides a relation between the enthalpy, pressure, temperature, and composition

$$H = H(T,p,x_i) \tag{8}$$

which is coupled with equations (5), (6), (7) and an equation for the molecular weight of the gas

$$\overline{M} = \left(\sum_i y_i\right)^{-1} \tag{9}$$

Normal-Shock Conditions

The conditions behind the normal shock are computed with the following inputs: the temperature, pressure, velocity, and gas composition ahead of the shock wave, an initial estimate for the temperature behind the shock, and the density ratio ρ_1/ρ_2 across the shock.

The initial estimate of ρ_1/ρ_2 is used in equations (5) and (6) to obtain ΔH_a and p_2. This value of p_2, an initial estimate of T_2 (which is equal to $T(1)$), and the gas composition ahead of the shock are used with equation (8) in the equilibrium program to obtain $H(1)$, a first estimate for H_2. (The free-stream conditions (T_1, p_1, x_i) are used directly in the equilibrium program to compute H_1.) The iteration technique used for

finding T_2 is the Newton-Raphson technique. To begin the iteration the first point $T(1)$ is the initial T_2 estimate with the second point arbitrarily chosen as $T(2) = T(1) + 10$. The term $\Delta H_{b(2)}$ which is equal to $H(2) - H_1$ determined from the equilibrium program when $T_2 = T(2)$ is now compared to ΔH_a (determined from eq. (5)) through the convergence criterion,

$$\left| \frac{\Delta H_a - \Delta H_{b(n)}}{\Delta H_a} \right| \leqq \tau = 10^{-5} \tag{10}$$

If the convergence criterion is not satisfied, a correction to T_2 is obtained, as noted previously, by the Newton-Raphson technique,

$$T_{n+1} = T_n - \frac{f(T_n)}{f'(T_n)} \tag{11}$$

where the functional relationship is written as

$$f(T_n) = \Delta H_a - (\Delta H_b)_n \tag{12}$$

and the first derivative with respect to temperature is

$$f'(T_n) = \frac{(\Delta H_b)_n - (\Delta H_b)_{n-1}}{T_n - T_{n-1}} \tag{13}$$

The quantity $(\Delta H_b)_n$ refers to the value of ΔH_b calculated from the nth estimate value of T_2. The temperature is repeatedly corrected until the convergence criterion is satisfied.

A second estimate for ρ_1/ρ_2 is obtained from equation (7) by using the conditions behind the shock that satisfied the convergence criterion. This estimate of ρ_1/ρ_2 is used in equations (5) and (6) to obtain new estimates for ΔH_a and p_2. This new estimate for p_2 and the previous estimate for T_2 are used to obtain a new ΔH_b, and T_2 is corrected until the convergence criterion is satisfied. The process of obtaining better estimates for ρ_1/ρ_2 and T_2 is continued until a given T_2, p_2, and ρ_1/ρ_2 satisfy equations (5), (6), (7), and the convergence criterion. (A flow diagram for the computation of the normal shock conditions is given in appendix B.) This procedure yields values of T_2, p_2, H_2, U_2, ρ_2, $(S/R)_2$, and the equilibrium gas composition.

Stagnation Conditions

The requirements at the stagnation point are

$$H_s = H_2 + \frac{1}{2} U_2^2 \tag{14}$$

and

$$\left(\frac{S}{R}\right)_s = \left(\frac{S}{R}\right)_2 \tag{15}$$

Briefly, the calculation procedure is as follows. Equation (14) is used to obtain H_s, the stagnation enthalpy. By using the pressure behind the shock wave p_2 and an initial arbitrary estimate for the stagnation temperature $T_2 + 10$, a value of the enthalpy is calculated through the equilibrium program. This enthalpy is compared with H_s through the convergence criterion defined by ϵ. (ϵ is initially set equal to 0.01, and during the iteration procedure, it is reduced to τ before the convergence is satisfied.)

$$\left|\frac{H_s - H}{H_s}\right| \leqq \epsilon \tag{16}$$

Better estimates for the temperature are obtained with the relation

$$\Delta T = \frac{H_s - H_n}{\dfrac{H_n - H_{n-1}}{T_n - T_{n-1}}} \tag{17}$$

where H_n is the value of the enthalpy calculated from the nth estimate of the temperature. This process is repeated until the convergence criterion is satisfied for a given temperature. This temperature and a new estimate for the stagnation pressure $(p_2 + \Delta p)$, where initially $\Delta p = 0.1p_2$ and for subsequent corrections

$$\Delta p = \frac{(S/R)_s - (S/R)_n}{\dfrac{(S/R)_n - (S/R)_{n-1}}{p_n - p_{n-1}}} \tag{18}$$

are then used in the equilibrium program to calculate S/R. Better estimates for p are obtained until the convergence criterion

$$\left|\frac{(S/R)_s - S/R}{(S/R)_s}\right| \leqq \epsilon \tag{19}$$

is satisfied. This estimate for the stagnation pressure and the last best estimate for the stagnation temperature are used in the equilibrium program to compute H. The value of H is compared by equation (16) with H_s. If the convergence criterion is not satisfied, the temperature is corrected. This separate iteration on the temperature and pressure is repeated until, for a given T and p, both equations (16) and (19) are satisfied. (The

flow diagram for the computation of the stagnation-point condition is given in appendix B.) This temperature T_s and pressure p_s are used to calculate the density and the gas composition at the stagnation point.

Local Conditions Over a Body

The inviscid flow at the outer edge of the boundary layer is considered to be isentropic. The normalized pressure distribution p_e/p_s, a required input, and the stagnation pressure are used to compute the local pressure. For each pressure the method of calculation, given in flow diagram form in appendix B, consists of an iteration on the temperature until the convergence criterion of equation (19) is satisfied. The corrections to the temperature are given by

$$\Delta T = \frac{(S/R)_s - (S/R)_n}{\dfrac{(S/R)_{n-1} - (S/R)_n}{T_n - T_{n-1}}} \tag{20}$$

The initial estimate for the temperature is arbitrarily chosen to be $T_s - 10$. When the convergence criterion is satisfied, the equilibrium gas composition, the density, enthalpy, velocity, and the derivative of the velocity with respect to the pressure are determined. The last term is obtained from the inviscid momentum equation for any x and is normalized in the program with the free-stream ρU product as

$$(\rho U)_1\left(\frac{dU}{dp}\right)_e = -\frac{(\rho U)_1}{(\rho U)_e} \tag{21}$$

This parameter is important since it can be used to determine the local velocity gradient $\left(\frac{dU}{dx}\right)_e$ if the pressure distribution over the body is known. The local velocity gradient is an important parameter in aerodynamic heat-transfer and shear-stress calculations. (See ref. 1.) Equation (21) does not apply at the stagnation point, but the stagnation-point velocity gradient can be determined by

$$\left(\frac{dU}{dx}\right)_s \approx \frac{1}{R_{eff}}\sqrt{\frac{2p_s}{\rho_s}} \tag{22}$$

where R_{eff} is the "effective" nose radius (ref. 13).

RESULTS AND DISCUSSION

Normal-shock and stagnation-point solutions for an air model are shown in figures 1 to 6. Excellent agreement is shown between the results of the present program and those obtained in references 4 and 14.

Figures 7, 8, and 9 show isentropic flow solutions for the normalized density, temperature, and enthalpy, respectively. These parameters are shown as functions of an assumed pressure distribution for several velocities at an altitude of 150 000 ft (45.72 km). The faired manually computed results were obtained with the use of a Mollier diagram for air. (See ref. 3.)

Figure 10 shows a typical variation of the normalized derivative of the velocity with respect to the pressure as a function of the pressure distribution. These results were computed at an altitude of 150 000 ft (45.72 km) and a velocity of 30 000 ft/sec (9.144 km/sec). As noted, this term with the pressure gradient over the body can be used to compute the local velocity gradient.

Figure 11 shows a typical variation of the gas species in mole fractions based on isentropic flow with an assumed pressure distribution. The results were computed for an air model (double-ionized species being neglected) at an altitude of 150 000 ft (45.72 km) and a velocity of 30 000 ft/sec (9.144 km/sec). Also, some typical, normal-shock gas compositions computed for air with the present program are compared with the results of references 4 and 14 in table I at altitudes of 50 000 ft (15.24 km) and 250 000 ft (76.2 km).

Figure 12 shows isentropic flow solutions for the normalized density, temperature, and enthalpy as functions of a pressure distribution based on an assumed Martain atmosphere $\left[\text{VM-7}\left(x_{CO_2} = 0.282;\ X_{N_2} = 0.718\right), \text{ref. } 15\right]$. The data were computed at a velocity of 15 200 ft/sec (4.64 km/sec) at an altitude of 300 000 ft (91.44 km) where $T_1 = 200^\circ$ K and $p_1 = 9.39$ dynes/cm^2. Also, the associated normal shock and stagnation-point values are given in the figure. The gas species in mole fractions for the conditions given in figure 12 are presented in figure 13 as a function of a normalized pressure distribution.

CONCLUDING REMARKS

A program for the calculation of local, blunt-body conditions and the accompanying normal-shock and stagnation-point conditions from given free-stream conditions has been developed. For the calculation of these conditions, the program combines the normal-shock relations and a general thermochemical equilibrium program with the assumption of isentropic flow and a known pressure distribution. Therefore, the local, blunt-body conditions and the corresponding heating rates and shear stress values can now be computed from known free-stream values and a pressure distribution over the body for arbitrary reacting gas mixtures.

Excellent correlations are obtained with existing solutions for an air model, and results for the normal-shock, stagnation-point, and local conditions based on an assumed

Martian atmosphere are presented. Also, the necessary program inputs and program listing with a sample input and output case are given in the appendixes of the paper.

The program was developed for the IBM 7094 electronic computer.

Langley Research Center,
National Aeronautics and Space Administration,
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129-01-03-02-23.

APPENDIX A

INPUT IDENTIFICATION

The input is loaded by using the Fortran IV namelist. The input symbols are as follows:

$NAM1

ISPEC	ordered list of integers selected from preceding list, for species desired behind normal shock
N	number of species
JMOL	ordered list of integers to correspond to components included in specie list
M	number of integers in JMOL
YSTO	non-zero mole numbers, y_i, as guess for composition behind shock
AMC	cold molecular weight of gas
PR	pressure ratios $\left(p_{local}/p_{stagnation}\right)$ for body expansion
NPR	number of pressure ratios (≤ 10)
TAU	convergence criteria – normally 1.E-5

$NAM2

p_1	free-stream pressure, atm
T_1	free-stream temperature, ^oK
U_1	free-stream velocity, ft/sec
T_2	guess temperature behind normal shock, ^oK
R1OR2	guess density ratio behind normal shock, ρ_1/ρ_2

One card of identification, columns 1 to 60, follows last data card.

The thermodynamic data for the program are on tape, as listed in reference 9, and are read and selected according to the ISPEC and JMOL lists by subroutine Tape.

APPENDIX A

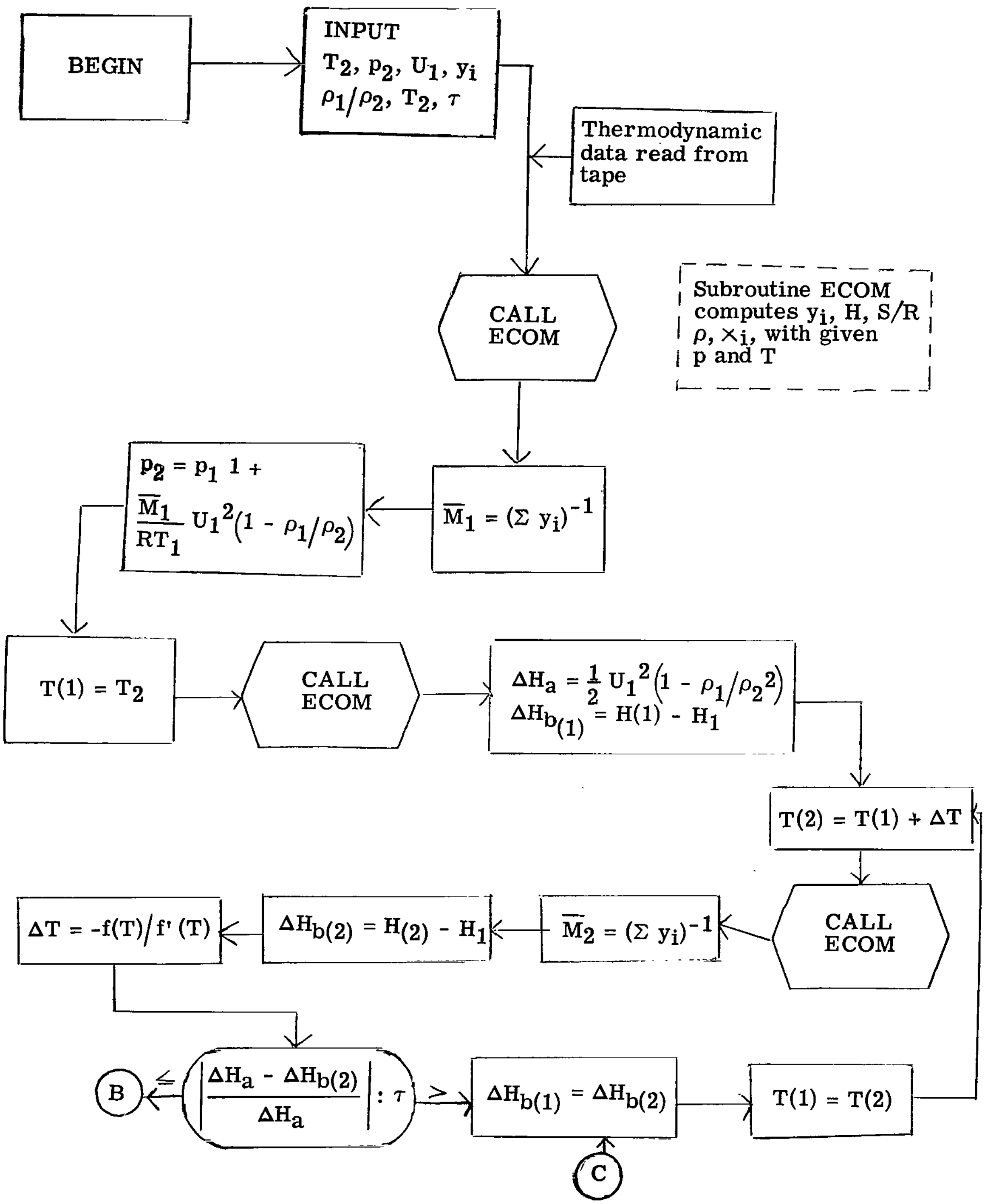
Listing of Species

ISPEC	Species	ISPEC	Species
1	e	21	O_2^-
2	N	22	NO
3	N^+	23	NO^+
4	N^{++}	24	C_2
5	O	25	CO
6	O^+	26	CO^+
7	O^{++}	27	CN
8	O^-	28	CN^-
9	C	29	H_2
10	C^+	30	OH
11	C^{++}	31	H_2O
12	C^-	32	CO_2
13	A	JMOL	Elements
14	A^+		
15	A^{++}	1	N
16	H	2	O
17	N_2	3	C
18	N_2^+	4	A
19	O_2	5	H
20	O_2^+	6	e

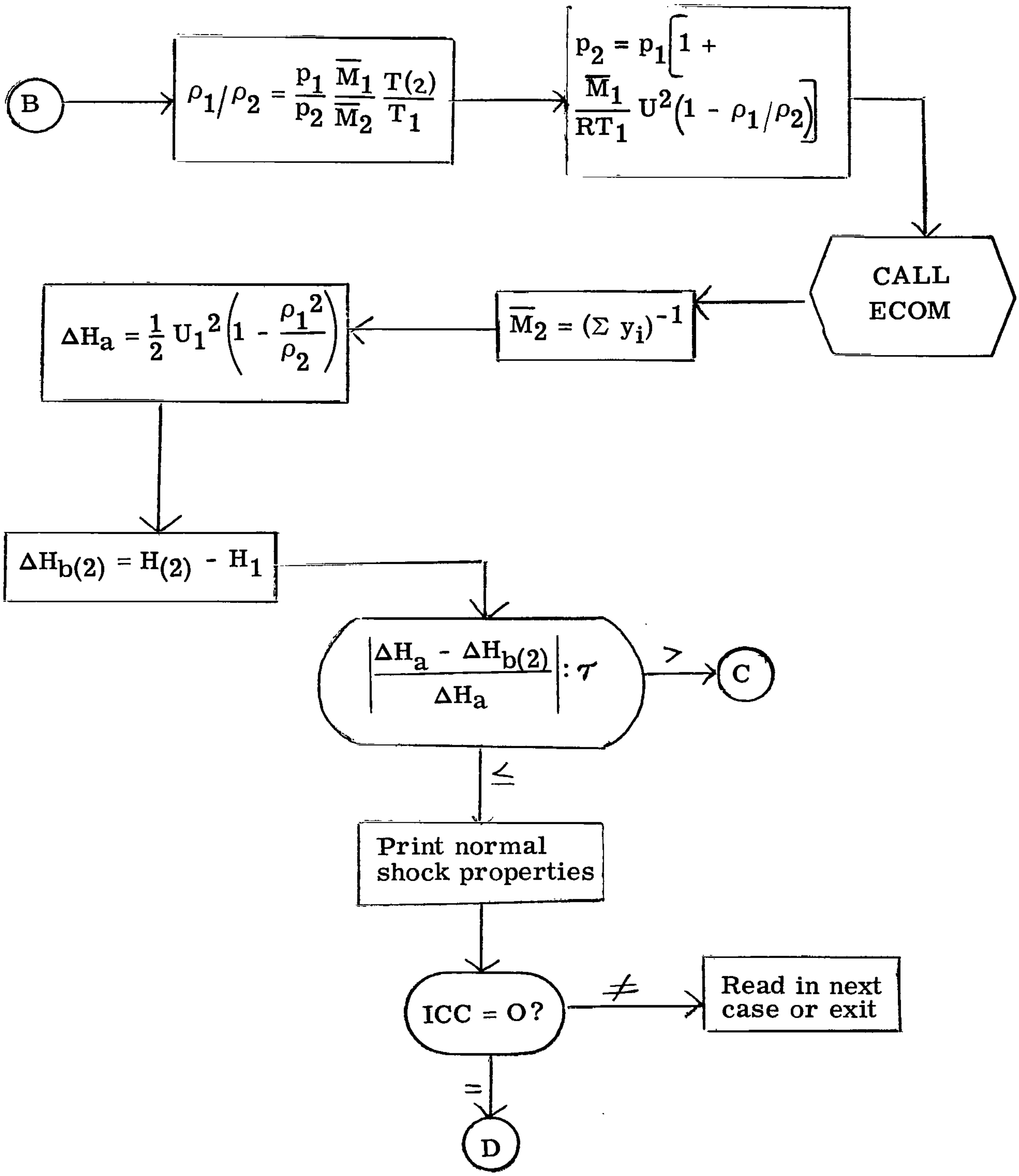
APPENDIX B

FLOW DIAGRAMS

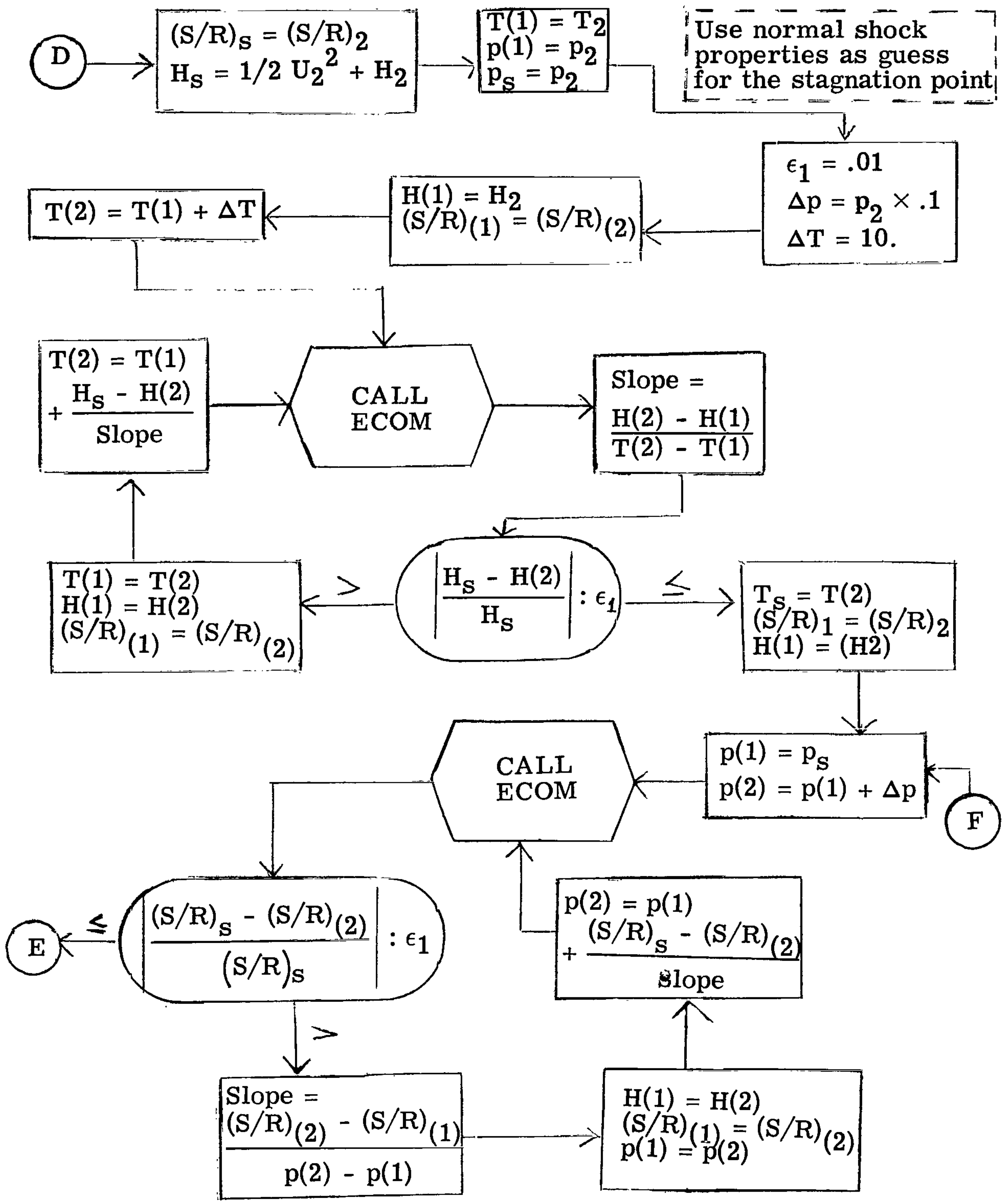
The flow diagram for the normal-shock solution is



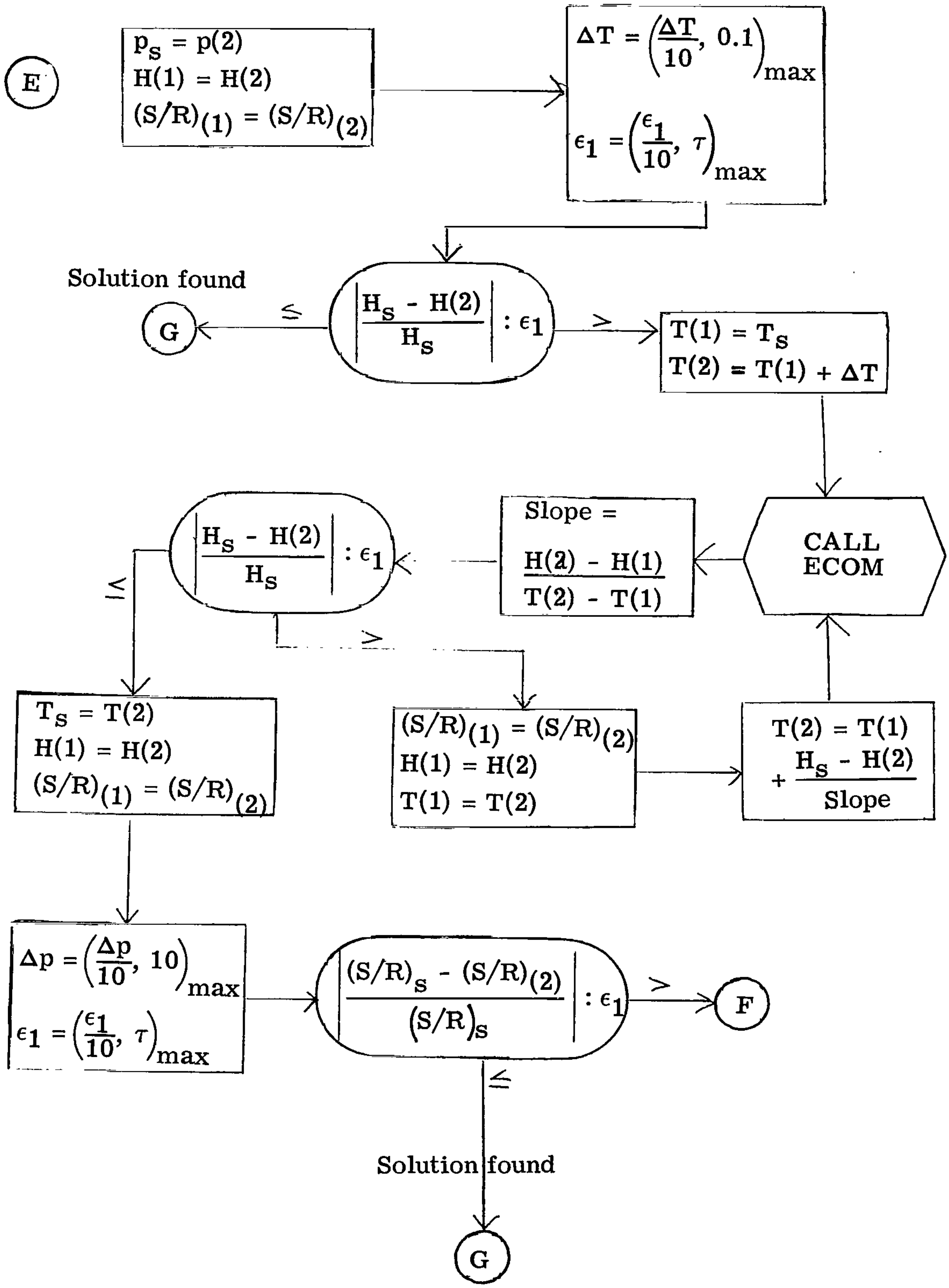
APPENDIX B


B
$\rho_1/\rho_2 = \frac{p_1}{p_2} \frac{\overline{M}_1}{\overline{M}_2} \frac{T(2)}{T_1}$
$p_2 = p_1\left[1 + \frac{\overline{M}_1}{RT_1} U^2(1 - \rho_1/\rho_2)\right]$
CALL ECOM
$\overline{M}_2 = (\Sigma\ y_i)^{-1}$
$\Delta H_a = \frac{1}{2} U_1^2\left(1 - \frac{\rho_1^2}{\rho_2}\right)$
$\Delta H_{b(2)} = H_{(2)} - H_1$
$\left|\frac{\Delta H_a - \Delta H_{b(2)}}{\Delta H_a}\right| : \tau$
>
C
≤
Print normal shock properties
ICC = O?
≠
Read in next case or exit
=
D

The flow diagram for the stagnation-point solution is



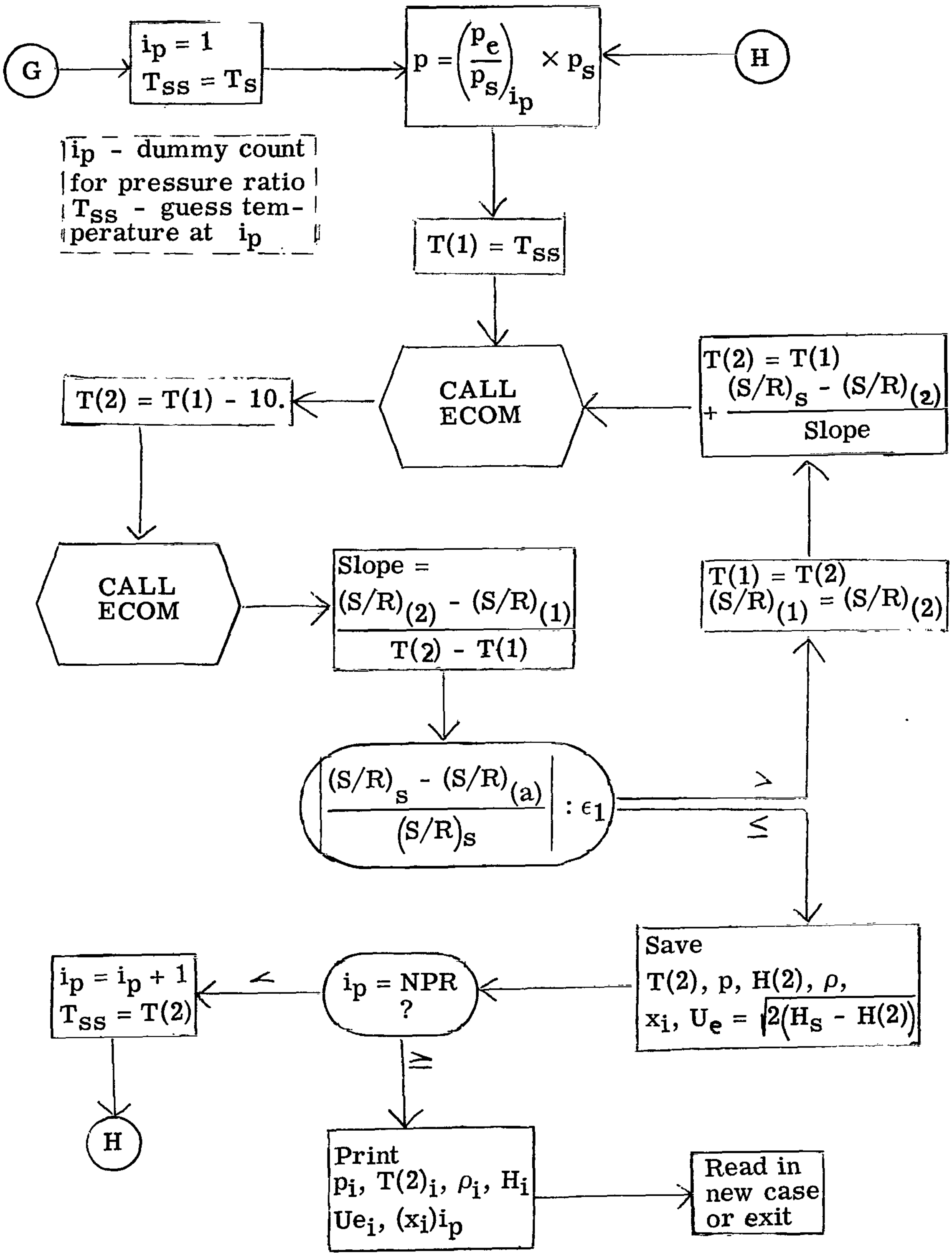
APPENDIX B



E
$p_s = p(2)$
$H(1) = H(2)$
$(S/R)_{(1)} = (S/R)_{(2)}$
$\Delta T = \left(\frac{\Delta T}{10}, 0.1\right)_{max}$
$\epsilon_1 = \left(\frac{\epsilon_1}{10}, \tau\right)_{max}$
Solution found
G
$\leq$
$\left|\frac{H_s - H(2)}{H_s}\right| : \epsilon_1$
$>$
$T(1) = T_s$
$T(2) = T(1) + \Delta T$
CALL ECOM
Slope = $\frac{H(2) - H(1)}{T(2) - T(1)}$
$\left|\frac{H_s - H(2)}{H_s}\right| : \epsilon_1$
$\leq$
$>$
$T_s = T(2)$
$H(1) = H(2)$
$(S/R)_{(1)} = (S/R)_{(2)}$
$(S/R)_{(1)} = (S/R)_{(2)}$
$H(1) = H(2)$
$T(1) = T(2)$
$T(2) = T(1) + \frac{H_s - H(2)}{\text{Slope}}$
$\Delta p = \left(\frac{\Delta p}{10}, 10\right)_{max}$
$\epsilon_1 = \left(\frac{\epsilon_1}{10}, \tau\right)_{max}$
$\left|\frac{(S/R)_s - (S/R)_{(2)}}{(S/R)_s}\right| : \epsilon_1$
$>$
F
$\leq$
Solution found
G

APPENDIX B

The flow diagram for the local flow solution is



APPENDIX C

PROGRAM LISTING

Program

The program listing is as follows:

```
$IBFTC P1248   LIST
      DIMENSION DHB(2),T(2),RHO(2)
      DIMENSIONSR(2),P(2),XSAVE(35,10),TSAVE(10),PSAVE(10),
     1HSAVE(10),DSAVE(10),ID1(10)
      DIMENSION X(35),XS(35),H(2)
      DIMENSION Y(35)
      DIMENSION USAVE(10),SSAVE(10)
      DIMENSION DUDP(10)
C
C      INPUT
C
      COMMON ISPEC(35),JMOL(10),N,M,AMC,T1,P1,U1,
     1YSTO(35),T2,R1OR2,TAU,PR(10),NPR,EPS,ICC
      COMMON/BLOCK/ICODE(35),F(35),CAPM(35),DHFO(35),L(35),G(30,35),
     1SMLE(30,35),CAPLAM(30,35),OMEG(5,30,35),A(10,35),CONR,CONPRF,
     2CONNO,CONH,CONK,PI,EPS1,NIT,EPS2,IC1
      NAMELIST/NAM1/ISPEC,JMOL,N,M,AMC,YSTO,TAU,PR,NPR,ICC/NAM2/T1,
     1P1,U1,T2,R1OR2,ICC
      ICC=0
      DELP=10000.
      READ(5,NAM1)
C
C     SUBROUTINE TAPE SELECTS FROM TAPE THE DATA FOR EACH OF THE SPECIES
C       CONSIDERED
C
      CALL TAPE(N,ISPEC,M,JMOL)
      WRITE (6,100)
  100 FORMAT(50H1 PROGRAM FOR COMPUTATION OF LOCAL FLOW PROPERTIES
     114X,9HP.N. 1248,10X,5H(LRC)//
     230H   JANE KEMPER FOR VINCENT ZOBY)
    1 READ(5,NAM2)
    5 READ(5,113)ID1
  113 FORMAT(10A6)
      WRITE(6,112) ID1
  112 FORMAT(17H1 FREESTREAM DATA///1H ,10A6)
      WRITE (6,114)U1,T1,P1
  114 FORMAT(///12H   VELOCITY =E15.8,5X,13HTEMPERATURE =E15.8,5X,
     110HPRESSURE =E15.8,5X,9HDENSITY =E15.8)
      DELT=10.
      NCOUNT=0
C
      DO 9 I=1,N
    9 Y(I)=YSTO(I)
C     COMPUTE H1
      P1=P1*1.01325E6
      U1=U1*3048.E-2
      DT2=1.
C
      ICELL=4
      CALL ECOM(T1,P1,Y,H1,X,ICELL,RHO1,SR(1))
```

APPENDIX C

```
C
      CAPMI=0.
      DO 10 I=1,N
   10 CAPMI=CAPMI+Y(I)
      CAPMI=1./CAPMI
C
   11 T(1)=T2
   20 P2=P1*(1.+CAPMI/(CONR*T1)*U1**2*(1.-R1OR2))
   21 ICELL=0.
      CALL ECOM(T(1),P2,Y,H2,X,ICELL,RHO(1),SR(1))
      IF(ICELL)29,29,28
   28 WRITE(6,302)
  302 FORMAT(//38H X(I) WOULD NOT CONVERGE FOR THIS CASE)
      GO TO 165
   29 DHA=.5*U1**2*(1.-R1OR2**2)
      DHB(1)=H2-H1
      T(2)=T(1)+DT2
  285 ICELL=0
      CALL ECOM(T(2),P2,Y,H2,X,ICELL,RHO(2),SR(2))
      CAPM2=0.
      DO 30 I=1,N
   30 CAPM2=CAPM2+Y(I)
      CAPM2=1./CAPM2
      IF(ICELL)31,31,28
   31 DHB(2)=H2-H1
      TEST=-(DHB(2)-DHA)/DHA
      DT2=(DHA-DHB(2))/((DHB(2)-DHB(1))/(T(2)-T(1)))
   32 IF(ABS(TEST)-TAU)40,40,35
   35 T(1)=T(2)
      DHB(1)=DHB(2)
      T(2)=T(1)+DT2
      IF(T(2))36,36,37
   36 T2=T2-(T2-T1)/2.
      GO TO 11
   37 IF(NIT-NCOUNT)300,300,51
   51 NCOUNT=NCOUNT+1
      GO TO 285
C
   40 R1OR2=P1/P2*CAPMI/CAPM2*T(2)/T1
      P2=P1*(1.+CAPMI/(CONR*T1)*U1**2*(1.-R1OR2))
      ICELL=0
      CALL ECOM(T(2),P2,Y,H2,X,ICELL,RHO(2),SOR2)
      IF(ICELL.NE.0) GO TO 28
      CAPM2=0
      DO 41 I=1,N
   41 CAPM2=CAPM2+Y(I)
      CAPM2=1./CAPM2
      DHA=.5*U1**2*(1.-R1OR2**2)
      DHB(2)=H2-H1
      DT2=10.
      TEST=-(DHB(2)-DHA)/DHA
      IF(ABS(TEST)-TAU)60,60,35
  300 WRITE(6,301)NIT
  301 FORMAT(//32H THIS CASE NON-CONVERGENT AFTER I4,11H ITERATIONS)
   60 U2=R1OR2*U1
      HS=.5*U2**2+H2
      P2=P2/1.01325E6
      WRITE(6,220)
```

```
  220 FORMAT(25H0 NORMAL SHOCK PROPERTIES)
      WRITE(6,114)U2,T(2),P2,RHO(2)
      WRITE(6,223) (ICODE(I),X(I),I=1,N)
  223 FORMAT(//4X,35HCOMPOSITION OF GAS (MOLE FRACTIONS)//
     1(11X,A3,3X,E15.8))
      WRITE(6,222)H2,SOR2
  222 FORMAT(//2X,10HENTHALPY =E15.8,17X,9HENTROPY =E15.8)
      WRITE (6,208)
C
C     LET HS = STAGNATION ENTHALPY AND SORS = STAGNATION ENTROPY
      IF(ICC-1) 75,165,75
   75 CONTINUE
C
      SORS=SOR2
C
C     LET TEMPERATURE BEHIND SHOCK BE FIRST ESTIMATE
C         OF STAGNATION
      TA1=TAU
      EPS=.01
      T(1)=T(2)
      H(1)=H2
      P(1)=P2*1.01325E6
      PS=P(1)
      DELP=PS*.1
      SR(1)=SOR2
C
      T(2)=T(1)+DELT
C
  110 CALL ECOM(T(2),P(1),Y,H(2),X,ICELL,RHO,SR(2))
      IF(ICELL)105,105,28
C
  105 SLOPE=(H(2)-H(1))/(T(2)-T(1))
C
      IF(ABS((HS-H(2))/HS)-EPS)115,115,111
  111 T(1)=T(2)
      H(1)=H(2)
      SR(1)=SR(2)
      T(2)=T(1)+(HS-H(2))/SLOPE
      GO TO 110
C
C     TS IS FINAL TEMP. ON CONSTANT PRESSURE CURVE.
C        THIS NOW BECOMES CONSTANT FOR PRESSURE
C        ITERATION.
C
  115 TS=T(2)
C
C      BEGIN CONSTANT TEMPERATURE ITERATION
C
  116 H(1)=H(2)
      SR(1)=SR(2)
      P(1)=PS
      P(2)=P(1)+DELP
  117 CALL ECOM(TS,P(2),Y,H(2),X,ICELL,RHO,SR(2))
C
      IF(ICELL)175,175,28
  175 SLOPE=(SR(2)-SR(1))/(P(2)-P(1))
C
```

```
      IF(ABS((SORS-SR(2))/SORS)-EPS)120,120,118
  118 DP=(SORS-SR(2))/SLOPE
      H(1)=H(2)
      SR(1)=SR(2)
      P(1)=P(2)
      P(2)=P(1)+DP
      GO TO 117
C
C     PS IS FINAL PRESSURE ON CONSTANT TEMPERATURE
C        CURVE.  THIS NOW BECOMES CONSTANT FOR
C       TEMPERATURE ITERATION IF SOLUTION HAS NOT
C       BEEN FOUND.
C
  120 PS=P(2)
      H(1)=H(2)
      SR(1)=SR(2)
      IF(DELT.GT..1) DELT=DELT/10.
      IF(EPS.GT.TA1) EPS=EPS/10.
C
      IF(ABS((HS-H(2))/HS)-TAU) 126,126,121
C
C      BEGIN CONSTANT PRESSURE ITERATION
C
  121 CONTINUE
      T(1)=TS
      T(2)=T(1)+DELT
C
  122 CALL ECOM(T(2),PS,Y,H(2),X,ICELL ,RHO,SR(2))
C
      SLOPE=(H(2)-H(1))/(T(2)-T(1))
C
      IF(ABS((HS-H(2))/HS)-EPS)125,125,123
  123 DT=(HS-H(2))/SLOPE
      SR(1)=SR(2)
      H(1)=H(2)
      T(1)=T(2)
      T(2)=T(1)+DT
      GO TO 122
C
  125 TS=T(2)
      IF(DELP.GT.10.) DELP=DELP/10.
      IF(EPS.GT.TA1) EPS=EPS/10.
C
      IF(ABS((SORS-SR(2))/SORS)-TAU) 126,126,116
C
C     SOLUTION FOUND
C
  126 PS=PS/CONPRF
      TS=TS
  130 HS=H(2)
      DS=RHO
      SORS=SR(2)
      US=0.
      DDS=0.
      DO 132 I=1,N
  132 XS(I)=X(I)
C
      TSS=TS
```

APPENDIX C

```
C
      IF(NPR.EQ.0) GO TO 155
C     BODY EXPANSION
C
      DO 150 I=1,NPR
      P=PR(I)*PS*CONPRF
C
C      LET FIRST ESTIMATE OF TEMPERATURE BE STAGNATION TEMPERATURE
C
      T(1)=TSS
      CALL ECOM(T(1),P,Y,H(1),X,ICELL,RHO,SR(1))
      T(2)=T(1)-10.
  133 CALL ECOM(T(2),P,Y,H(1),X,ICELL,RHO,SR(2))
C
      SLOPE=(SR(2)-SR(1))/(T(2)-T(1))
C
      IF(ABS((SORS-SR(2))/SORS)-EPS)135,135,134
C
  134 DT=(SORS-SR(2))/SLOPE
      T(1)=T(2)
      SR(1)=SR(2)
      T(2)=T(1)+DT
      GO TO 133
C
  135 PSAVE(I)=P/1.01325E6
      TSS=T(2)
      TSAVE(I)=T(2)
      HSAVE(I)=H(1)
      DSAVE(I)=RHO
      IF((H(1)-HS).GT.1.E-7) GO TO 1355
      USAVE(I)=SQRT(2.*(HS-H(1)))
      UE=USAVE(I)
      DUDP(I)=RHO1*U1*(-1./(RHO*UE))
 1356 SSAVE(I)=SR(2)
      DO 136 J=1,N
  136 XSAVE(J,I)=X(J)
      GO TO 150
 1355 USAVE(I)=0.
      GO TO 1356
  150 CONTINUE
C
C     WRITE STAGNATION POINT BODY DATA
C
      IF(NPR-6)155,155,160
  155 WRITE(6,200)
  200 FORMAT(1H1,33X,40HSTAGNATION POINT AND BODY EXPANSION DATA// )
      WRITE(6,201) (PR(I),I=1,NPR)
  201 FORMAT(5H P/PS,15X,5H1.000,7X,5(4X,F7.3,6X),4X,F7.3)
      WRITE(6,202) PS,(PSAVE(I),I=1,NPR)
  202 FORMAT(/15H PRESSURE(ATM) ,6(E15.8,2X),E15.8)
      WRITE(6,203) TS,(TSAVE(I),I=1,NPR)
  203 FORMAT(15H TEMPERATURE   ,6(E15.8,2X),E15.8)
      WRITE(6,204) HS,(HSAVE(I),I=1,NPR)
  204 FORMAT(15H ENTHALPY      ,6(E15.8,2X),E15.8)
      WRITE(6,2222) SORS,(SSAVE(I),I=1,NPR)
 2222 FORMAT(15H ENTROPY       ,6(E15.8,2X),E15.8)
      WRITE(6,205) DS,(DSAVE(I),I=1,NPR)
```

```
 205 FORMAT(15H DENSITY        ,6(E15.8,2X),E15.8)
     WRITE(6,210) US,(USAVE(I),I=1,NPR)
 210 FORMAT(15H VELOCITY       6(E15.8,2X),E15.8)
     WRITE(6,211) DDS,(DUDP(I),I=1,NPR)
 211 FORMAT(15H DU/DP          6(E15.8,2X),E15.8)
     WRITE(6,206)
 206 FORMAT(/33X,32HGAS COMPOSITION (MOLE FRACTIONS)/)
     DO 157 J=1,N
 157 WRITE(6,207)ICODE(J),XS(J),(XSAVE(J,I),I=1,NPR)
 207 FORMAT(6X,A3,6X,E15.8,2X,E15.8,2X,E15.8,2X,E15.8,2X,E15.8,2X,
    1E15.8,2X,E15.8)
     GO TO 165
 160 WRITE(6,200)
     WRITE(6,201) (PR(I),I=1,6)
     WRITE(6,202) PS,(PSAVE(I),I=1,6)
     WRITE(6,203) TS,(TSAVE(I),I=1,6)
     WRITE(6,204) HS,(HSAVE(I),I=1,6)
     WRITE(6,2222) SORS,(SSAVE(I),I=1,6)
     WRITE(6,205) DS,(DSAVE(I),I=1,6)
     WRITE(6,210) US,(USAVE(I),I=1,6)
     WRITE(6,211) DDS,(DUDP(I),I=1,6)
     WRITE(6,206)
     DO 158 J=1,N
 158 WRITE(6,207) ICODE(J),XS(J),(XSAVE(J,I),I=1,6)
C
     WRITE(6,209)
 209 FORMAT(1H1,33X,48HSTAGNATION POINT AND BODY EXPANSION DATA (CONT.)
    1)
     WRITE(6,215)  (PR(I),I=7,NPR)
 215 FORMAT(5H PS/P,10X,6(4X,F7.3,6X),4X,F7.3)
     WRITE(6,202)  (PSAVE(I),I=7,NPR)
     WRITE(6,203)  (TSAVE(I),I=7,NPR)
     WRITE(6,204)  (HSAVE(I),I=7,NPR)
     WRITE(6,2222) (SSAVE(I),I=7,NPR)
     WRITE(6,205)  (DSAVE(I),I=7,NPR)
     WRITE(6,210) (USAVE(I),I=7,NPR)
     WRITE(6,211) (DUDP(I),I=7,NPR)
     WRITE(6,206)
     DO 63 J=1,N
  63 WRITE(6,207)ICODE(J),(XSAVE(J,I),I=7,NPR)
C
 165 WRITE(6,208)
 208 FORMAT(//132H ----------------------------------------------------
    1-----------------------------------------------------------------
    2-------------)
     P1=P1/1.01325E6
     U1=U1/30.48
     GO TO 1
     END
```

APPENDIX C

```
$IBFTC ECOM     LIST
      SUBROUTINE ECOM(T,P,Y,H,X,ICELL,RHO,SOR)
C
C     SUBROUTINE WHICH, GIVEN A TEMPERATURE AND PRESSURE, COMPUTES
C     THE THERMODYNAMIC EQUILIBRIUM PROPERTIES OF A GAS DESCRIBED BY
C     THE INPUT.
C
      DIMENSION SMALE(30,35),X(35)
      DIMENSION E(35),Q(35),CAPFI(35),R(10,10),B(10),
     3TEMPS(10),BSUM(11,1),ABLOCK(11,11),PTEMP(35),ZETA(35),
     4ZETAPR(35),ALAM(35),
     5IPIVOT(11),INDEX(11,2),DQINT(35),QINT(30,35)
      DIMENSION Y(35)
C
      COMMON/BLOCK/ICODE(35),F(35),CAPM(35),DHFO(35),L(35),G(30,35),
     1SMLE(30,35),CAPLAM(30,35),OMEG(5,30,35),A(10,35),CONR,CONPRF,
     2CONNO,CONH,CONK,PI,EPS1,NIT,EPS2,IC1
      COMMON ISPEC(35),JMOL(10),N,M,AMC,T1,P1,U1,
     1YSTO(35),T2,R1OR2,TAU,PR(10),NPR,EPS,ICC
      EQUIVALENCE(SMLE(1,1),SMALE(1,1)),(ICODE(1),CODE(1))
      POP=P/CONPRF
C
      PI=3.14159
      C=2.99793E10
      NCOUNT=0
      LTEST=LTEST
      N2=N
   34 TK=CONK*T
      RT=CONR*T
      DO 999 J=1,M
      B(J)=0.0
      DO 999 I=1,N
      B(J)=B(J)+A(J,I)*Y(I)
  999 CONTINUE
  346 YBAR=0.0
      DO 347 I=1,N
  347 YBAR=YBAR+Y(I)
      DO 40 I=1,N
      TEMP1=0
      LEND=L(I)
      DO 37 L1=1,LEND
      IF(F(I))31,35,31
   31 PROD=1.
      DO 33 IC=1,IC1
      IF(OMEG(IC,L1,I))32,33,32
   32 PROD=PROD*(1.-EXP(-CONH*C*OMEG(IC,L1,I)/TK))
   33 CONTINUE
      FF=F(I)
      PART=(T/(CAPLAM(L1,I)*PROD))**FF
      GO TO 36
   35 PART=1.
   36 QINT(L1,I)=PART*G(L1,I)*EXP(-CONH*C*SMALE(L1,I)/TK)
   37 TEMP1=TEMP1+QINT(L1,I)
      Q(I)=(SQRT(2.*PI/CONH*TK/(CONH*CONNO)*CAPM(I))**3)*TK/CONPRF*TEMP1
      IF(Y(I)/YBAR)38,38,39
   38 CAPFI(I)=0
      GO TO 40
   39 CAPFI(I)=Y(I)*(ALOG(POP      )+ALOG(Y(I)/YBAR)-ALOG(Q(I))+DHFO(I)
     1/RT)
```

```
   40 CONTINUE
      IF(ICELL-4)396,95,396
  396 DO 50 J=1,M
      DO 50 K=1,M
      R(K,J)=0.0
      DO 50 I=1,N
   50 R(K,J)=R(K,J)+A(J,I)*A(K,I)*Y(I)
C
C     SET UP MATRIX FOR SOLUTION OF EQUATIONS
C
      DO 60 J=1,M
      TEMPS(J)=0.0
      DO 55 I=1,N
   55 TEMPS(J)=TEMPS(J)+A(J,I)*CAPFI(I)
      BSUM(J,1)=B(J)+TEMPS(J)
C
C     CONSTANT TERMS IN BSUM BLOCK
C
      DO 56 K=1,M
      K1=K+1
   56 ABLOCK(J,K1)=R(K,J)
C
C     PI TERMS IN ABLOCK IN COLUMNS 2 THROUGH N+1
C
   60 ABLOCK(J,1)=B(J)
C
C     (X/Y) TERMS IN FIRST COLUMN
C
      M1=M+1
      ABLOCK(M1,1)=0.0
      DO 61 K=1,M1
      K1=K+1
   61 ABLOCK(M1,K1)=B(K)
      BSUM(M1,1)=0.0
      DO 62 I=1,N
   62 BSUM(M1,1)=BSUM(M1,1)+CAPFI(I)
C
C     MATINV EXPECTS AN M+1 BY M+1 MATRIX
C
      CALL MATINV(ABLOCK(1,1),M1,BSUM(1,1),1,DETERM,IPIVOT,INDEX,11,0)
C
C     RETURN WITH ANSWERS IN BSUM
C
      ZETAP=BSUM(1,1)*YBAR
      ZERO=0.
      NEG=0.0
      DO 70 I=1,N
      PTEMP(I)=0.0
      DO 65 J=1,M
      J1=J+1
   65 PTEMP(I)=PTEMP(I)+BSUM(J1,1)*A(J,I)*Y(I)
      ZETA(I)=-CAPFI(I)+Y(I)*BSUM(1,1)+PTEMP(I)
C
C     TEST FOR NEGATIVE OR ZERO ZETA
C
   68 IF(ZETA(I))69,695,70
   69 PIECE=-Y(I)/(ZETA(I)-Y(I))
      IF(PIECE)691,692,691
```

```
  691 NEG=NEG+1
      ALAM(NEG)=PIECE
      GO TO 70
  692 Y(I)=0
      ZERO=1.
      GO TO 70
  695 IF(Y(I))69,70,69
   70 CONTINUE
C
C     FIND GREATEST NEGATIVE ZETA-Y
C
      IF(ZERO)700,700,698
  698 IF(NCOUNT-NIT)699,100,100
  699 NCOUNT=NCOUNT+1
      GO TO 346
  700 IF(NEG-1)78,71,73
   71 ALAMPR=.999999*ALAM(1)
      GO TO 745
   73 ARG1=ALAM(1)
      DO 74 I=2,NEG
   72 ARG2=ALAM(I)
      ARG1=AMIN1(ARG1,ARG2)
   74 CONTINUE
      ALAMPR=.999999*ARG1
  745 IIC=0
   75 ZETAP=0
      DO 76 I=1,N
      ZETAPR(I)=Y(I)+ALAMPR*(ZETA(I)-Y(I))
   76 ZETAP=ZETAP+ZETAPR(I)
      DLAM=0
      DO 77 I=1,N
      IF(ZETAPR(I)/ZETAP)77,77,765
  765 DLAM=DLAM+(ZETA(I)-Y(I))*(ALOG(POP      )-ALOG(Q(I))+DHFO(I)/RT+ALO
     1G(ZETAPR(I)/ZETAP))
   77 CONTINUE
      IF(DLAM)81,81,80
   80 IF(IIC-3)805,81,81
  805 IIC=IIC+1
      ALAMPR=ALAMPR*.9
      GO TO 75
   78 ALAMPR=1.
      GO TO 745
C
C     CONVERGENCE TEST FOR Y(I)S
C
   81 IF(ALAMPR-.70)83,815,815
  815 DO 82 I=1,N
      IF(ZETAPR(I))813,816,813
  813 REL=Y(I)-ZETAPR(I)
      IF(ABS(REL)-EPS1)818,818,83
  818 REL=ZETAPR(I)/Y(I)-1.
      IF(ABS(REL)-EPS2)82,82,83
  816 IF(Y(I))817,82,817
  817 GO TO 83
   82 CONTINUE
C
C     Y(I)S CONVERGE
C
```

APPENDIX C

```
      DO 800  I=1,N
  800 Y(I)=ZETAPR(I)
      GO TO 95
C
C     NON-CONVERGENCE OF Y(I)S
C
   83 NCOUNT=NCOUNT+1
      IF(NCOUNT-NIT)84,100,100
   84 DO 85  I=1,N
   85 Y(I)=ZETAPR(I)
C
C     REPEAT WITH NEW Y(I)S AND NO. OF ITERATIONS LESS THAN NIT
C
      GO TO 346
   95 DO 201  I=1,N
  201 X(I)=Y(I)*CAPM(I)
      YBAR=0.0
      CAPMI=0
      DO 2026  I=1,N
      YBAR=YBAR+Y(I)
 2026 CAPMI=CAPMI+X(I)/CAPM(I)
      CAPMI=1.0/CAPMI
      Z=AMC/CAPMI
      ESUM=0
      DO 2029  I=1,N
      QSUM=0
      DQINT(I)=0
      LEND=L(I)
      DO 2028 L1=1,LEND
      SUM=0
      DO 2027  IC=1,IC1
      HOOTK=CONH*C*OMEG(IC,L1,I)/TK
      IF(OMEG(IC,L1,I))2000,2027,2000
 2000 SUM=SUM+HOOTK/(EXP(HOOTK)-1.)
 2027 CONTINUE
      DQINT(I)=DQINT(I)+QINT(L1,I)*(F(I)/T*(1.+SUM)+SMALE(L1,I)*CONH*C
     1/(TK*T))
 2028 QSUM=QSUM+QINT(L1,I)
      E(I)=1./CAPM(I)*(1.5*RT+RT*T/QSUM*DQINT(I)+DHFO(I))
 2029 ESUM=ESUM+X(I)*E(I)
      HOZRT=CAPMI*ESUM/(CONR*T)+1.
      H=HOZRT*CONR*T*Z/AMC
      TK=T*CONK
      FSUM=0
      DO 2040  I=1,N
 2033 IF(Y(I))2034,2034,2035
 2034 CAPFI(I)=0
      GO TO 2040
 2035 CAPFI(I)=Y(I)*(ALOG(POP      )+ALOG(Y(I)/YBAR)-ALOG(Q(I))+DHFO(I)
     1/RT)
 2040 FSUM=FSUM+CAPFI(I)
      SOZR=HOZRT-CAPMI*FSUM
      SOR=SOZR*Z
      RHO=P*CAPMI/RT
      OOZ=1.0/Z
      DO 300  I=1,N
```

```
  300 X(I)=X(I)*CAPMI/CAPM(I)
      ICELL=0
      RETURN
  100 ICELL=1
      RETURN
      END
```

```
$IBFTC TAPE
      SUBROUTINE TAPE(N,ISPEC,J,JMOL)
C
C
C     SUBROUTINE TAPE SELECTS THERMODYNAMIC DATA FROM TAPE
C
      COMMON/BLOCK/ICODE(35),F(35),CAPM(35),DHFO(35),L(35),G(30,35),
     1SMLE(30,35),CAPLAM(30,35),OMEG(5,30,35),A(10,35),CONR,CONPRF,
     2CONNO,CONH,CONK,PI,EPS1,NIT,EPS2,IC1
      DIMENSION BLOCK(150),LBLOCK(35),ISPEC(35),JMOL(10),
     1OBL(5,30)
      READ(9) (LBLOCK(I),I=1,35)
      DO 1 IC=1,N
      ISP=ISPEC(IC)
    1 ICODE(IC)=LBLOCK(ISP)
C
      READ(9) (BLOCK(I),I=1,35)
      DO 2 IC=1,N
      ISP=ISPEC(IC)
    2 F(IC)=BLOCK(ISP)
C
      READ(9) (BLOCK(I),I=1,35)
      DO 3 IC=1,N
      ISP=ISPEC(IC)
    3 CAPM(IC)=BLOCK(ISP)
C
      READ(9) (BLOCK(I),I=1,35)
      DO 4 IC=1,N
      ISP=ISPEC(IC)
    4 DHFO(IC)=BLOCK(ISP)
C
      READ(9) (LBLOCK(I),I=1,35)
      DO 5 IC=1,N
      ISP=ISPEC(IC)
    5 L(IC)=LBLOCK(ISP)
C
      IC=1
      DO 6 I=1,35
      READ (9) (BLOCK(IL),IL=1,30)
      IF(ISPEC(IC)-I)6,55,6
```

```
   55 DO 56 LI=1,30
   56 G(LI,IC)=BLOCK(LI)
      IC=IC+1
    6 CONTINUE
C
      IC=1
      DO 7 I=1,35
      READ (9) (BLOCK(IL),IL=1,30)
      IF(ISPEC(IC)-I)7,65,7
   65 DO 66 LI=1,30
   66 SMLE(LI,IC)=BLOCK(LI)
      IC=IC+1
    7 CONTINUE
      IC=1
      DO 12I=1,35
      READ (9) (BLOCK(IL),IL=1,30)
      IF(ISPEC(IC)-I)12,13,12
   13 DO 125 LI=1,30
  125 CAPLAM(LI,IC)=BLOCK(LI)
      IC=IC+1
   12 CONTINUE
C
      IIC=1
      DO 8 I=1,35
      READ(9) ((OBL(IC,IL),IC=1,5),IL=1,30)
      IF(ISPEC(IIC)-I)8,75,8
   75 DO 76 LI=1,30
      DO 76 IC=1,5
   76 OMEG(IC,LI,IIC)=OBL(IC,LI)
      IIC=IIC+1
    8 CONTINUE
C
      IC=1
      DO 10I=1,35
      READ(9)(BLOCK(IJ),IJ=1,10)
      IF(ISPEC(IC)-I)10,85,10
   85 DO 9 IJ=1,J
      IJM=JMOL(IJ)
    9 A(IJ,IC)=BLOCK(IJM)
      IC=IC+1
   10 CONTINUE
C
      CONR=8.3146938E7
      CONPRF=1.01325E6
      CONNO=6.02322E23
      CONH=6.62517E-27
      CONK=1.38044E-16
      PI=3.14159
      NIT=300
      EPS1=1.E-6
      EPS2=.01
```

```
      IF(ISPEC(N)-32)14,15,14
   14 N1=N-1
      IF(ISPEC(N1)-31) 145,146,145
  145 IC1=1
      GO TO 20
  146 IC1=3
      GO TO 20
   15 IC1=4
   20 RETURN
      END
```

Comments on use of ECOM Subroutine

The program uses a routine MATINV to solve a matrix equation, $AX = B$ where A is a square coefficient matrix and B is a matrix of constant vectors. Reference to this routine is found in subroutine ECOM following statement 62. The calling sequence of this routine is shown and briefly described in order to allow replacement by a similar routine, if necessary.

CALL MATINV (ABLOCK(1,1), M1, BSUM(1,1), 1, DETERM, IPIVOT, INDEX, 11, 0)

ABLOCK – first location of matrix A

M1 – location of order of A, $1 < M1 \leqq 11$

BSUM – first location of B

1 – number of column vectors

DETERM – gives value of determinant (not used)

IPIVOT, INDEX – temporary storage

11 – maximum order of A

0 – factor used in computing determinant

At return to calling program, X is stored at BSUM.

APPENDIX D

SAMPLE INPUTS AND OUTPUTS

A sample input and a sample output are given in this appendix.

Sample Input

```
$DATA
 $NAM1
  PR(1)=.99,.9,.8,.7,.6,.5,.4,.3,.2,.1,NPR=10,
 AMC=        28.962,
 YSTO=       1.E-18,1.E-18,1.E-18,1.E-18,1.E-18,1.E-18,
             3.211E-4,1.E-18,2.69E-2,1.E-18,7.24E-3,1.E-18,
             1.E-18,1.E-18,1.E-18,
  JMOL=1,2,4,6,
 M=          4,
  ISPEC=1,2,3,5,6,8,13,14,17,18,19,20,21,22,23,
 N=          15,
   TAU=1.E-5$
 $NAM2
  P1=2.23E-4,T1=249.,U1=40000.,T2=12300.,R1OR2=.0615$
  SAMPLE CASE FOR AIR  AT 200,000FT.
```

Sample Output

```
FREESTREAM DATA

 SAMPLE CASE FOR AIR  AT 200,000FT.

VELOCITY = 0.40000000E 05    TEMPERATURE = 0.24900000E 03    PRESSURE = 0.22300000E-03    DENSITY =

NORMAL SHOCK PROPERTIES

VELOCITY = 0.74991244E 05    TEMPERATURE = 0.12343715E 05    PRESSURE = 0.43624694E 00    DENSITY = 0.51488102E-05

  COMPOSITION OF GAS (MOLE FRACTIONS)

        E-      0.17990338E 00
        N       0.49064710E 00
        N+      0.15244018E 00
        O       0.14657430E 00
        O+      0.26522893E-01
        O-      0.25254940E-05
        A       0.29216198E-02
        A+      0.91719370E-03
        N2      0.42063018E-04
        N2+     0.10724541E-04
        O2      0.95200257E-07
        O2+     0.13135691E-06
        O2-     0.34849522E-11
        NO      0.32409129E-05
        NO+     0.14647475E-04

ENTHALPY = 0.74290099E 12                 ENTROPY = 0.67451369E 02
```

STAGNATION POINT AND BODY EXPANSION DATA

P/PS	1.000	0.990	0.900	0.800	0.700	0.600	0.500
PRESSURE(ATM)	0.45140171E 00	0.44688769E 00	0.40626154E 00	0.36112136E 00	0.31598119E 00	0.27084102E 00	0.22570086E 00
TEMPERATURE	0.12383357E 05	0.12371338E 05	0.12258190E 05	0.12120495E 05	0.11967188E 05	0.11793714E 05	0.11592938E 05
ENTHALPY	0.74571493E 12	0.74484558E 12	0.73668040E 12	0.72673789E 12	0.71566997E 12	0.70314722E 12	0.68864702E 12
ENTROPY	0.67451122E 02	0.67451284E 02	0.67451352E 02	0.67451361E 02	0.67451514E 02	0.67451718E 02	0.67451230E 02
DENSITY	0.53028756E-05	0.52572803E-05	0.48436431E-05	0.43767379E-05	0.39010817E-05	0.34153399E-05	0.29177761E-05
VELOCITY	0.00000000E-38	0.41697756E 05	0.13442121E 06	0.19481810E 06	0.24513246E 06	0.29177975E 06	0.33783994E 06
DU/DP	0.00000000E-38	-0.17613590E 01	-0.59303694E 00	-0.45283693E 00	-0.40377164E 00	-0.38746510E 00	-0.39170465E 00

GAS COMPOSITION (MOLE FRACTIONS)

E-	0.18103860E 00	0.18067343E 00	0.17723863E 00	0.17300587E 00	0.16822970E 00	0.16274080E 00	0.15626631E 00
N	0.48880395E 00	0.48939726E 00	0.49497921E 00	0.50186497E 00	0.50964249E 00	0.51858996E 00	0.52915583E 00
N+	0.15339530E 00	0.15308827E 00	0.15019951E 00	0.14663261E 00	0.14259949E 00	0.13795477E 00	0.13246417E 00
O	0.14616213E 00	0.14629461E 00	0.14753717E 00	0.14906272E 00	0.15077723E 00	0.15273888E 00	0.15504163E 00
O+	0.26693497E-01	0.26638157E-01	0.26120404E-01	0.25488009E-01	0.24781766E-01	0.23979072E-01	0.23043328E-01
O-	0.25884612E-05	0.25698073E-05	0.23988638E-05	0.22017069E-05	0.19958095E-05	0.17797244E-05	0.15514247E-05
A	0.29069149E-02	0.29115307E-02	0.29548934E-02	0.30079672E-02	0.30673689E-02	0.31349293E-02	0.32135655E-02
A+	0.92639770E-03	0.92348078E-03	0.89617819E-03	0.86289164E-03	0.82583316E-03	0.78395288E-03	0.73561595E-03
N2	0.41727502E-04	0.41847232E-04	0.42983886E-04	0.44432898E-04	0.46133440E-04	0.48183625E-04	0.50755873E-04
N2+	0.10807855E-04	0.10785275E-04	0.10570905E-04	0.10308339E-04	0.10013599E-04	0.96781273E-05	0.92895192E-05
O2	0.96321737E-07	0.96018340E-07	0.93167982E-07	0.89760569E-07	0.86041897E-07	0.81941868E-07	0.77364895E-07
O2+	0.13345960E-06	0.13284658E-06	0.12716973E-06	0.12048883E-06	0.11333713E-06	0.10560910E-06	0.97152661E-07
O2-	0.36335750E-11	0.35899290E-11	0.32002132E-11	0.27749704E-11	0.23588800E-11	0.19536032E-11	0.15612857E-11
NO	0.32536860E-05	0.32511633E-05	0.32263195E-05	0.31955848E-05	0.31605238E-05	0.31201967E-05	0.30736785E-05
NO+	0.14654380E-04	0.14655702E-04	0.14666660E-04	0.14682487E-04	0.14702887E-04	0.14730637E-04	0.14771852E-04

STAGNATION POINT AND BODY EXPANSION DATA (CONT.)

PS/P	0.400	0.300	0.200	0.100
PRESSURE(ATM)	0.18056068E 00	0.13542051E 00	0.90280341E-01	0.45140170E-01
TEMPERATURE	0.11353716E 05	0.11054875E 05	0.10650144E 05	0.99955046E 04
ENTHALPY	0.67140461E 12	0.64992539E 12	0.62100801E 12	0.57499205E 12
ENTROPY	0.67451258E 02	0.67451319E 02	0.67451199E 02	0.67451323E 02
DENSITY	0.24055871E-05	0.18747974E-05	0.13183835E-05	0.72104105E-06
VELOCITY	0.38551350E 06	0.43769749E 06	0.49941350E 06	0.58433361E 06
DU/DP	-0.41635235E 00	-0.47053647E 00	-0.58643466E 00	-0.91643324E 00

GAS COMPOSITION (MOLE FRACTIONS)

E-	0.14840694E 00	0.13836519E 00	0.12439911E 00	0.10111340E 00
N	0.54199699E 00	0.55842575E 00	0.58130766E 00	0.61951096E 00
N+	0.12578319E 00	0.11722432E 00	0.10528689E 00	0.85326370E-01
O	0.15782247E 00	0.16135591E 00	0.16624105E 00	0.17434409E 00
O+	0.21922243E-01	0.20509776E-01	0.18574141E-01	0.15389212E-01
O-	0.13080570E-05	0.10452274E-05	0.75541206E-06	0.42269858E-06
A	0.33074495E-02	0.34247100E-02	0.35824901E-02	0.38310476E-02
A+	0.67851058E-03	0.60823576E-03	0.51582090E-03	0.37628723E-03
N2	0.54115846E-04	0.58867102E-04	0.66561842E-04	0.83602246E-04
N2+	0.88248227E-05	0.82461230E-05	0.74726890E-05	0.62715311E-05
O2	0.72122937E-07	0.65937853E-07	0.58247693E-07	0.47599765E-07
O2+	0.87721350E-07	0.76908837E-07	0.63910139E-07	0.46600355E-07
O2-	0.11843908E-11	0.82711779E-12	0.49614836E-12	0.20448302E-12
NO	0.30175448E-05	0.29482724E-05	0.28592205E-05	0.27412409E-05
NO+	0.14831539E-04	0.14928134E-04	0.15109437E-04	0.15581785E-04

REFERENCES

1. Beckwith, Ivan E.; and Cohen, Nathaniel B.: Application of Similar Solutions to Calculations of Laminar Heat Transfer on Bodies With Yaw and Large Pressure Gradients In High-Speed Flow. NASA TN D-625, 1961.
2. Lewis, Clark H.; and Burgess, Ernest G., III: Altitude-Velocity Tables and Charts for Imperfect Air. AEDC-TDR-64-214, U.S. Air Force, Jan. 1965. (Available from DDC as AD 454078.)
3. Feldman, Saul: Hypersonic Gas Dynamic Charts for Equilibrium Air. Res. Rept. 40, Avco-Everett Res. Lab., Jan. 1957.
4. Wittliff, Charles E.; and Curtis, James T.: Normal Shock Wave Parameters in Equilibrium Air. Rept. No. CAL-111 (Contract No. AF 33(616)-6579), Cornell Aeron. Lab. Inc., Nov. 1961.
5. Ziemer, Richard W.: Extended Hypervelocity Gas Dynamic Charts for Equilibrium Air. STL/TR-60-0000-09093 (Contract AF04(647-309), Space Technol. Labs.,Inc., Apr. 14, 1960.
6. Laird, J. D.; and Heron, K.: Shock Tube Gas Dynamic Charts. Part I: Equilibrium Argon-Free Air From 3000° K to 40,000° K. RAD-TM-64-12, Avco Corp., Apr. 10, 1964.
7. Grabau, Martin: A Method of Forming Continuous Empirical Equations for the Thermodynamic Properties of Air From Ambient Temperatures to 15,000° K, With Applications. AEDC-TN-59-102 (Contract No. AF40(600)-800), Arnold Eng. Dev. Center, Aug. 1959.
8. Lordi, J. A.; Mates, R. E.; and Moselle, J. R.: Computer Program for the Numerical Solution of Nonequilibrium Expansions of Reacting Gas Mixtures. Rept. No. AD-1689-A-6 (Contract No. NASr-109), Cornell Aeron. Lab., Inc., Oct. 1965.
9. Allison, Dennis O.: Calculations of Thermodynamic Properties of Gas Mixtures at High Temperatures. M.S. Thesis, Virginia Polytech. Inst., 1965.
10. White, W. B.; Johnson, S. M.; and Dantzig, G. B.: Chemical Equilibrium in Complex Mixtures. J. Chem. Phys., vol. 28, no. 5, May 1958, pp. 751-755.
11. Newman, Perry A.; and Allison, Dennis O.: Direct Calculation of Specific Heats and Related Thermodynamic Properties of Arbitrary Gas Mixtures With Tabulated Results. NASA TN D-3540, 1966.
12. Allison, Dennis O.: Calculation of Thermodynamic Properties of Arbitrary Gas Mixtures With Modified Vibrational-Rotational Corrections. NASA TN D-3538, 1966.

13. Zoby, Ernest V.; and Sullivan, Edward M.: Effects of Corner Radius on Stagnation-Point Velocity Gradients on Blunt Axisymmetric Bodies. NASA TM X-1067, 1965.

14. Marrone, Paul V.: Normal Shock Waves in Air: Equilibrium Composition and Flow Parameters for Velocities From 26,000 and 50,000 ft/sec. CAL Rept. No. AG-1729-A-2 (Contract NASr-119), Cornell Aeron. Lab., Inc., Aug. 1962.

15. Anon.: Comparative Studies of Conceptual Design and Qualification Procedures for a Mars Probe/Lander. Final Report. Volume III: Probe, Entry from Orbit – Book 1: System Design. AVSSD-0006-66-RR (Contract NAS 1-5224), AVCO Corp., May 11, 1966.

TABLE I.- TYPICAL COMPARISON OF GAS COMPOSITION IN MOLE FRACTIONS BEHIND NORMAL SHOCK

Species	Mole fraction behind normal shock for U_1 of –							
	2000 ft/sec (0.6096 km/sec)		15 000 ft/sec (4.57 km/sec)		30 000 ft/sec (9.145 km/sec)		50 000 ft/sec (15.24 km/sec)	
	Present method	Reference 4	Present method	Reference 4	Present method	Reference 14	Present method	Reference 14
	Altitude, 50 000 ft (15.24 km)							
N_2	7.809×10^{-1}	7.809×10^{-1}	6.27×10^{-1}	6.283×10^{-1}	8.764×10^{-2}	9.016×10^{-2}	1.218×10^{-4}	1.494×10^{-4}
O_2	2.097×10^{-1}	2.098×10^{-1}	1.11×10^{-2}	1.225×10^{-2}	1.316×10^{-4}	1.485×10^{-4}	4.389×10^{-6}	7.441×10^{-6}
A	9.3×10^{-3}	9.324×10^{-3}	7.909×10^{-3}	7.949×10^{-3}	5.063×10^{-3}	5.077×10^{-3}	1.779×10^{-3}	1.676×10^{-3}
NO	5.315×10^{-13}		5.467×10^{-2}	5.657×10^{-2}	5.089×10^{-3}	5.464×10^{-3}	4.516×10^{-5}	5.555×10^{-5}
N			1.951×10^{-2}	1.828×10^{-2}	6.689×10^{-1}	6.654×10^{-1}	3.957×10^{-1}	3.84×10^{-1}
O	2.061×10^{-32}	4.628×10^{-32}	2.797×10^{-1}	2.766×10^{-1}	2.226×10^{-1}	2.227×10^{-1}	1.182×10^{-1}	1.158×10^{-1}
e			5.414×10^{-5}	5.318×10^{-5}	5.259×10^{-3}	5.429×10^{-3}	2.418×10^{-1}	2.487×10^{-1}
N_2^+			2.59×10^{-8}	2.391×10^{-8}	3.155×10^{-4}	3.757×10^{-4}	1.036×10^{-4}	1.624×10^{-4}
O_2^+			1.982×10^{-7}	2.012×10^{-7}	3.916×10^{-6}	4.468×10^{-6}	5.824×10^{-6}	9.276×10^{-6}
NO^+			5.83×10^{-5}	5.673×10^{-5}	6.541×10^{-4}	7.595×10^{-4}	0.789×10^{-4}	1.084×10^{-4}
N^+			5.554×10^{-9}	4.712×10^{-9}	3.596×10^{-3}	3.598×10^{-3}	1.989×10^{-1}	2.05×10^{-1}
O^+			10.308×10^{-8}	9.604×10^{-8}	7.24×10^{-4}	7.407×10^{-4}	4.121×10^{-2}	4.203×10^{-2}
O^-			4.315×10^{-6}	3.877×10^{-6}	5.765×10^{-5}	7.146×10^{-5}	2.212×10^{-4}	4.284×10^{-4}
A^+			5.006×10^{-10}		2.31×10^{-5}	2.259×10^{-5}	1.765×10^{-3}	1.836×10^{-3}
O_2^-			1.783×10^{-7}		6.612×10^{-8}		2.64×10^{-8}	

Species	Mole fraction behind normal shock for U_1 of –							
	5000 ft/sec (1.52 km/sec)		15 000 ft/sec (4.57 km/sec)		30 000 ft/sec (9.145 km/sec)		50 000 ft/sec (15.24 km/sec)	
	Present method	Reference 4	Present method	Reference 4	Present method	Reference 14	Present method	Reference 14
	Altitude, 250 000 ft (72.20 km)							
N_2	7.808×10^{-1}	7.808×10^{-1}	5.879×10^{-1}	5.898×10^{-1}	3.184×10^{-3}	3.386×10^{-3}	8.032×10^{-7}	8.865×10^{-7}
O_2	2.096×10^{-1}	2.097×10^{-1}	7.189×10^{-5}	8.065×10^{-5}	2.908×10^{-7}	3.173×10^{-7}	3.434×10^{-9}	4.08×10^{-9}
A	9.301×10^{-3}	9.324×10^{-3}	7.44×10^{-3}	7.459×10^{-3}	4.624×10^{-3}	4.626×10^{-3}	1.098×10^{-3}	1.126×10^{-3}
NO	2.577×10^{-4}	2.5×10^{-4}	2.549×10^{-3}	2.658×10^{-3}	3.187×10^{-5}	3.424×10^{-5}	8.754×10^{-8}	9.884×10^{-8}
N	3.669×10^{-16}	3.172×10^{-16}	7.094×10^{-2}	6.716×10^{-2}	7.659×10^{-1}	7.658×10^{-1}	1.94×10^{-1}	1.951×10^{-1}
O	7.066×10^{-7}	6.616×10^{-7}	3.293×10^{-1}	3.328×10^{-1}	2.077×10^{-1}	2.078×10^{-1}	7.02×10^{-2}	7.004×10^{-2}
e			4.378×10^{-5}	4.257×10^{-5}	9.316×10^{-3}	9.158×10^{-3}	3.673×10^{-1}	3.669×10^{-1}
N_2^+			9.327×10^{-9}	8.979×10^{-9}	0.984×10^{-5}	1.112×10^{-5}	1.114×10^{-6}	1.428×10^{-6}
O_2^+			4.373×10^{-9}	4.633×10^{-9}	4.544×10^{-8}	4.971×10^{-8}	2.192×10^{-8}	2.605×10^{-8}
NO^+			4.36×10^{-5}	4.239×10^{-5}	6.965×10^{-5}	8.073×10^{-5}	1.645×10^{-6}	1.999×10^{-6}
N^+			1.458×10^{-8}	1.39×10^{-8}	7.557×10^{-3}	7.379×10^{-3}	3.024×10^{-1}	3.016×10^{-1}
O^+			1.586×10^{-7}	1.58×10^{-7}	1.66×10^{-3}	1.668×10^{-3}	5.311×10^{-2}	6.341×10^{-2}
O^-			3.865×10^{-9}	3.329×10^{-9}	1.008×10^{-7}	1.001×10^{-7}	4.087×10^{-7}	5.429×10^{-7}
A^+			1.824×10^{-10}		2.035×10^{-5}	1.889×10^{-5}	1.858×10^{-3}	1.832×10^{-3}
O_2^-			1.746×10^{-3}		2.391×10^{-6}		1.725×10^{-8}	

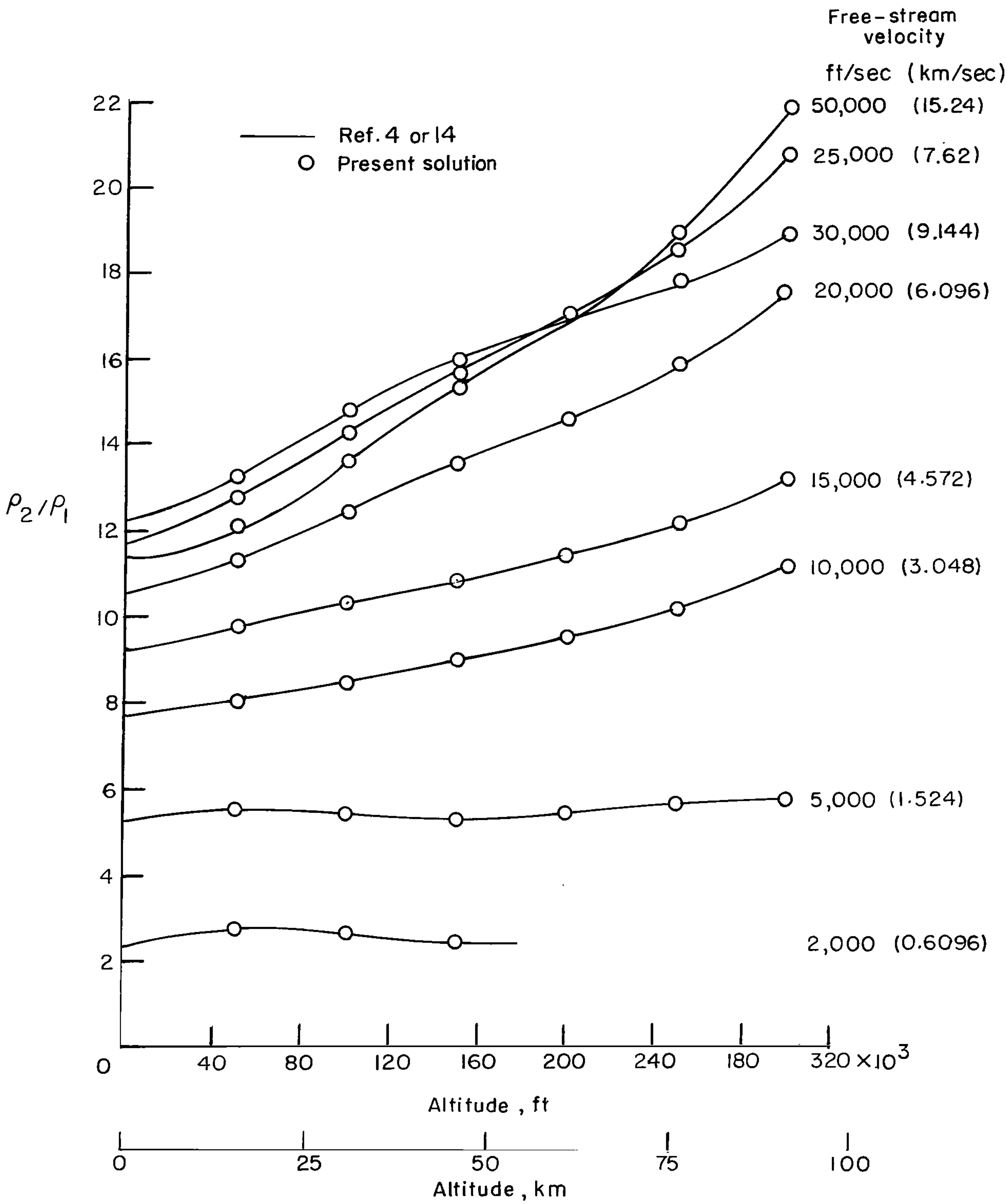


Figure 1.- Density ratio as a function of altitude.

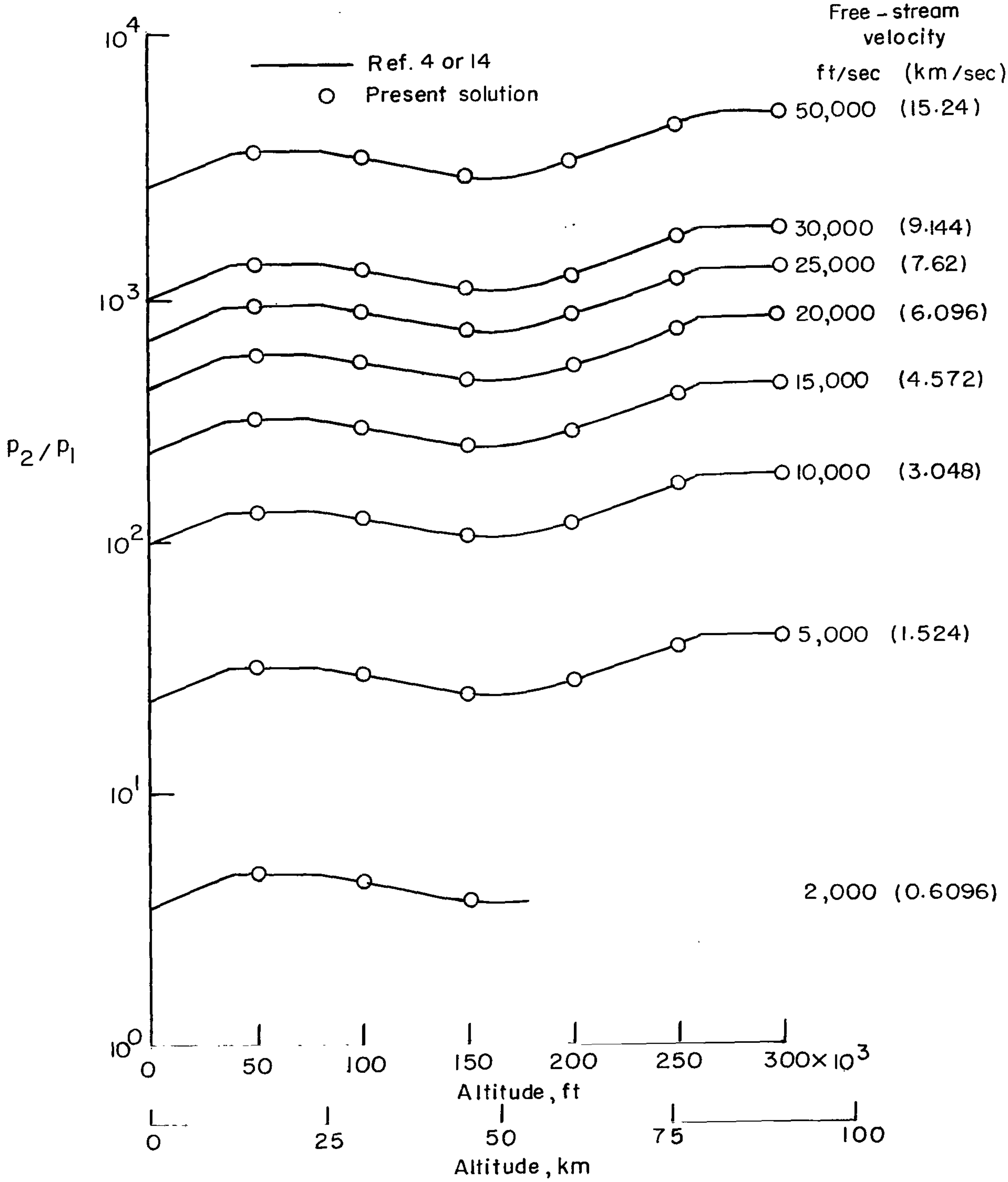


Figure 2.- Pressure ratio as a function of altitude.

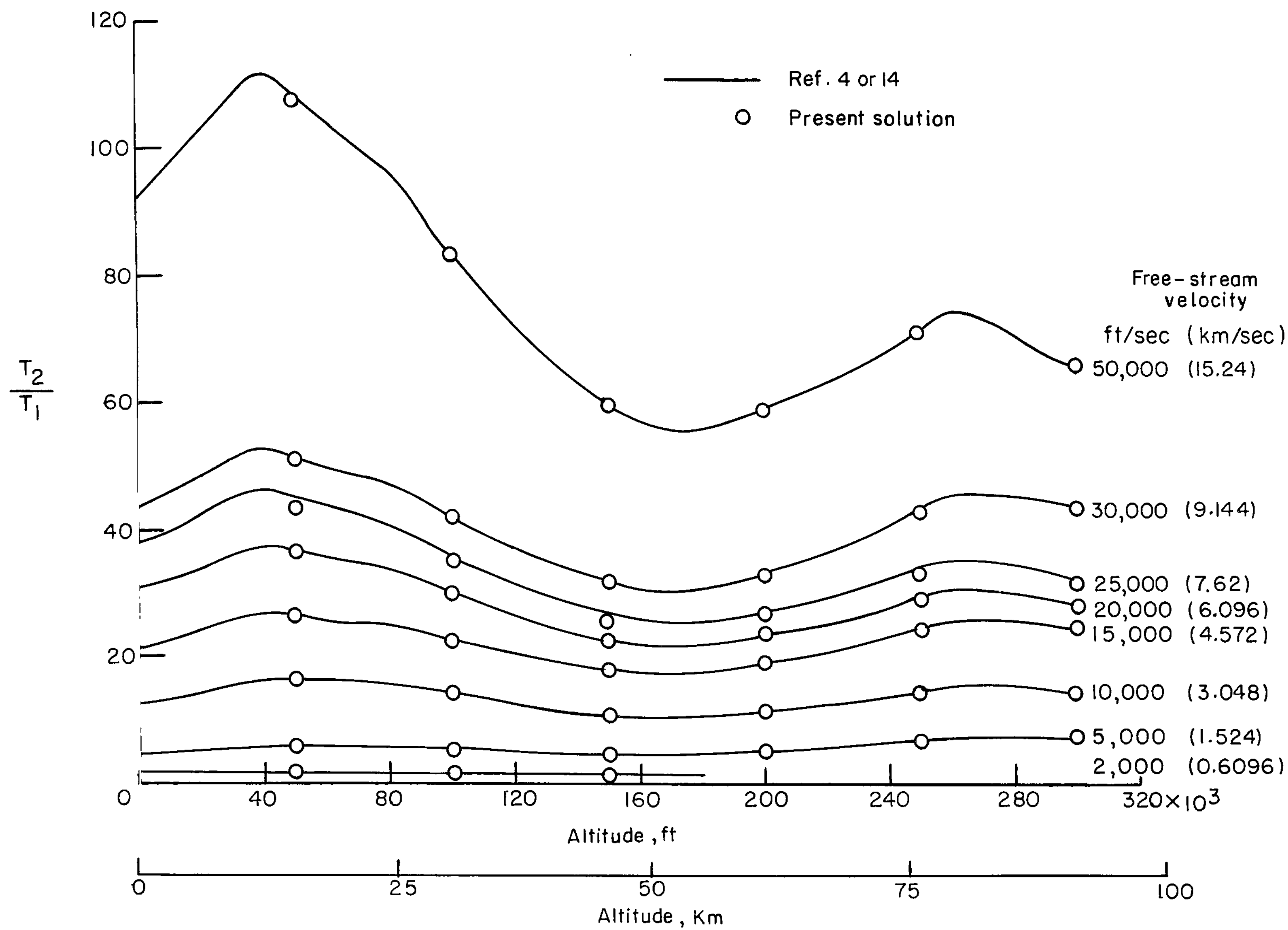


Figure 3.- Temperature ratio as a function of altitude.

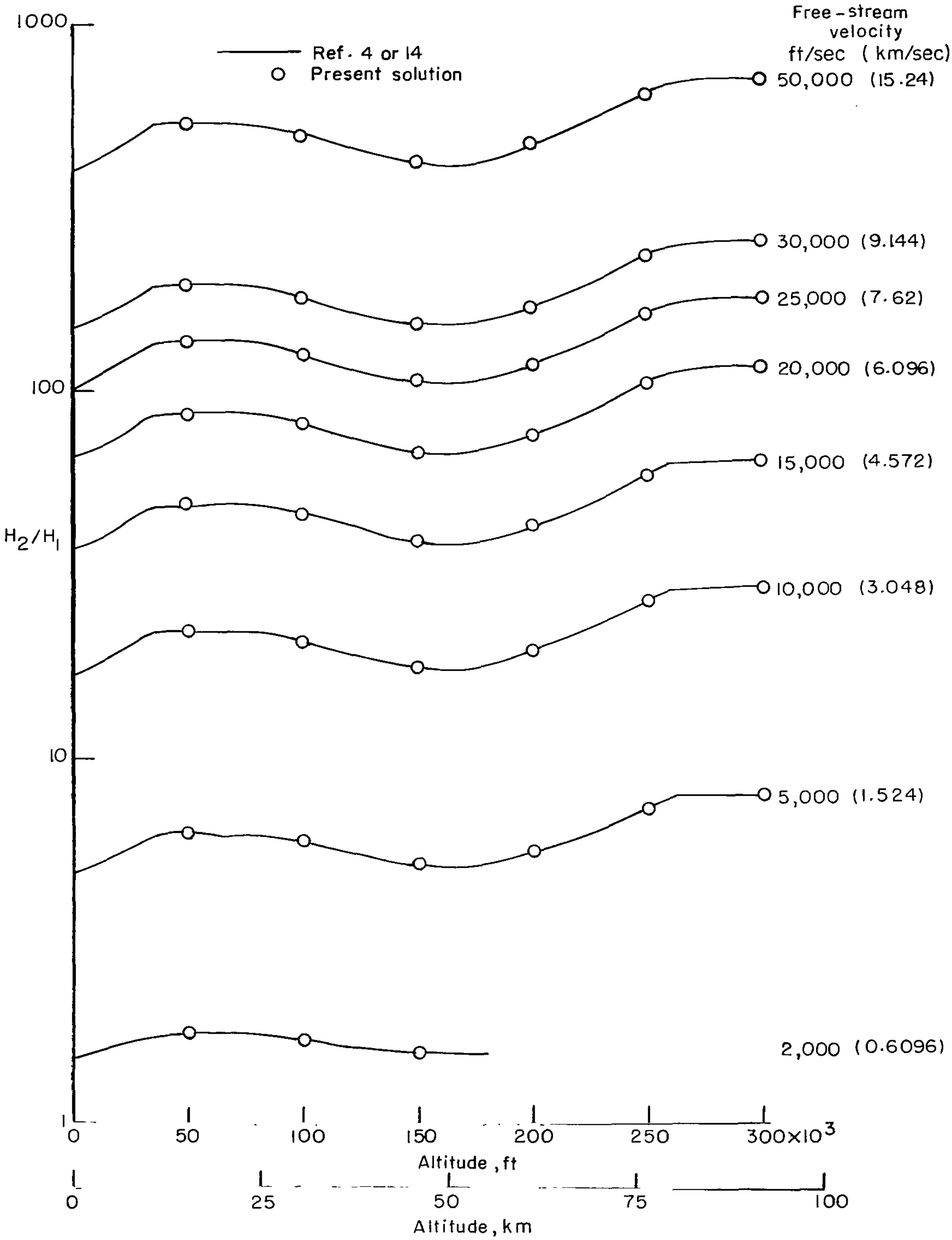


Figure 4.- Enthalpy ratio as a function of altitude.

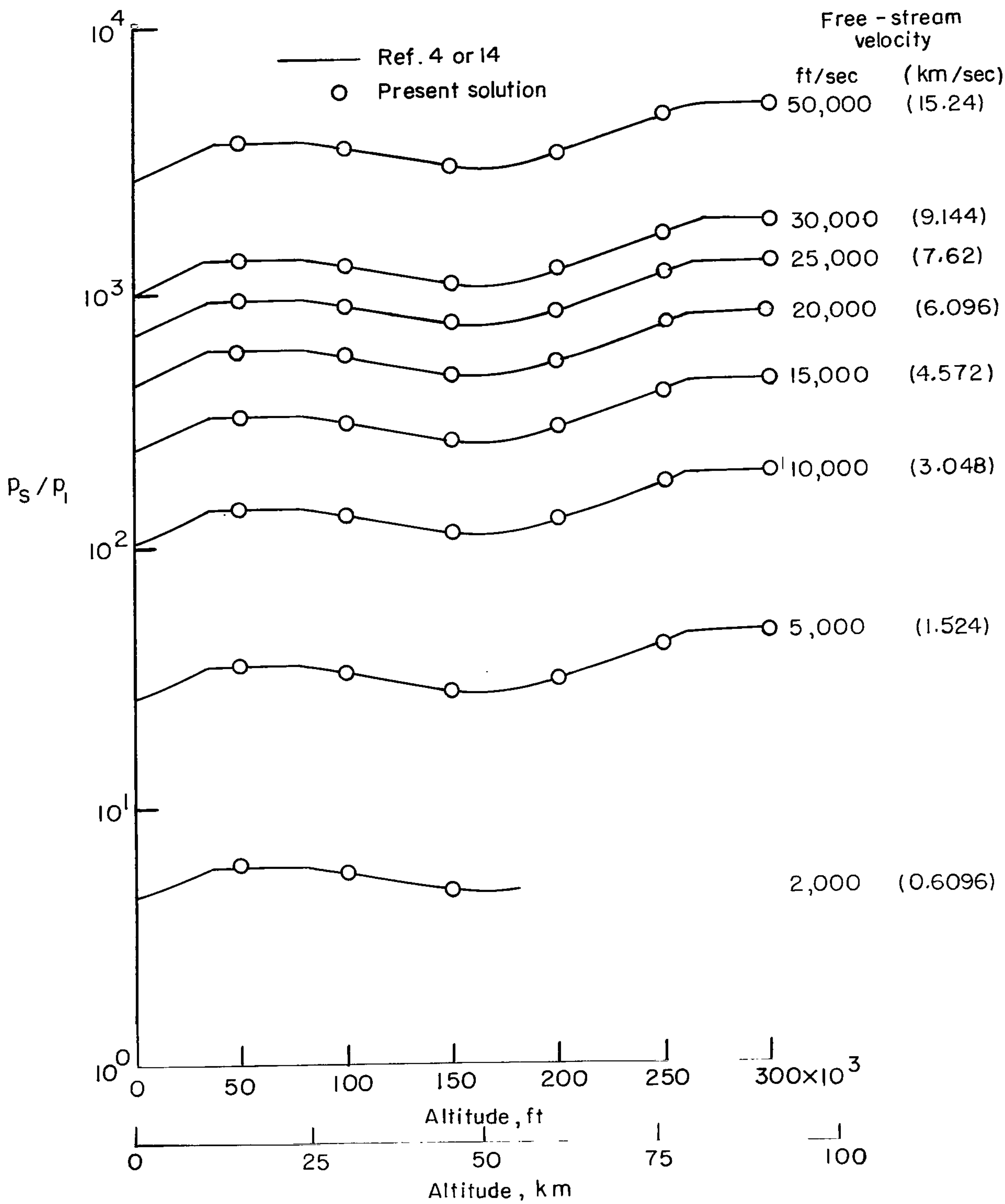


Figure 5.- **Stagnation-point** pressure ratio as a function of altitude.

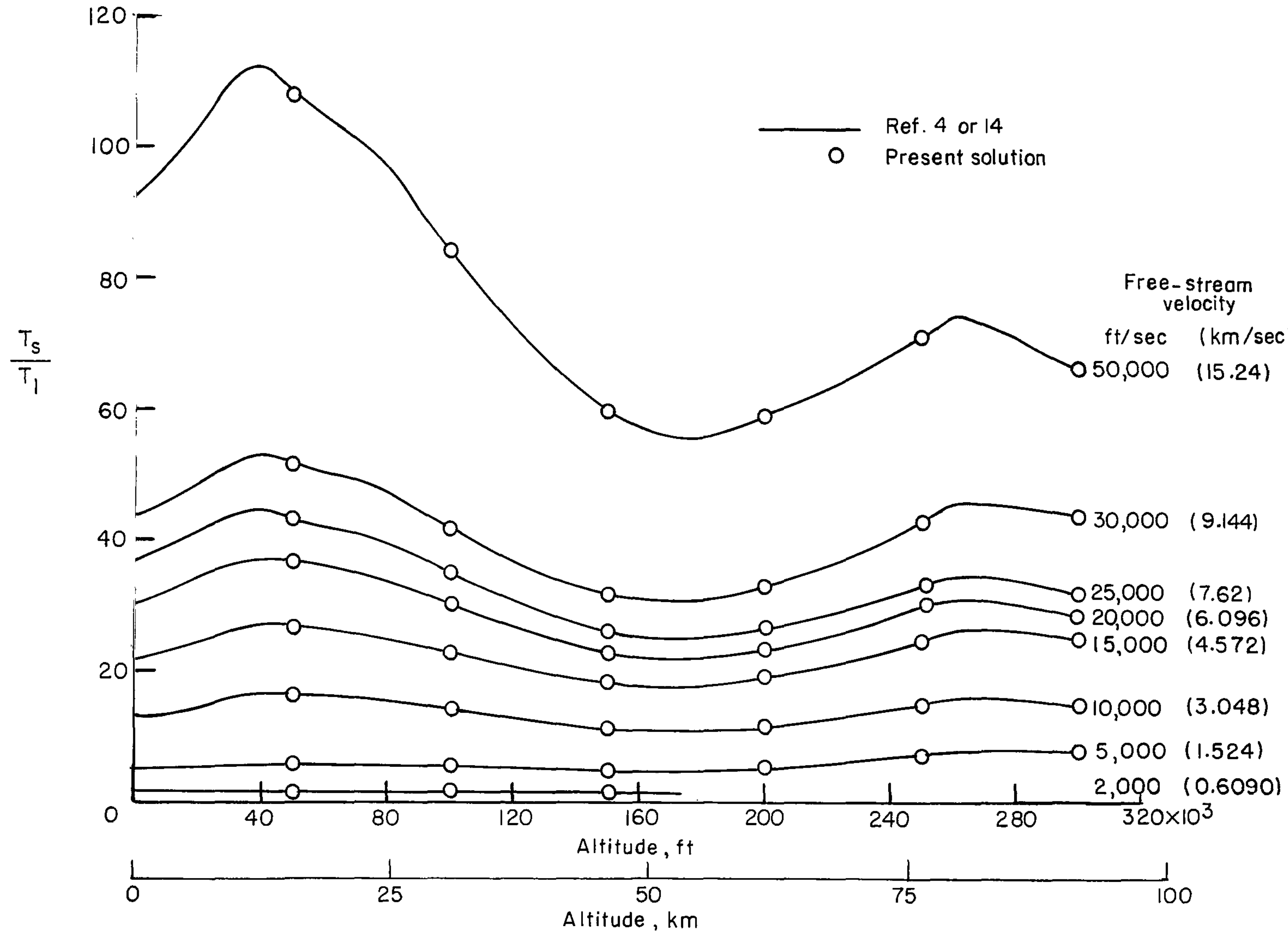


Figure 6.- Stagnation-point temperature as a function of altitude.

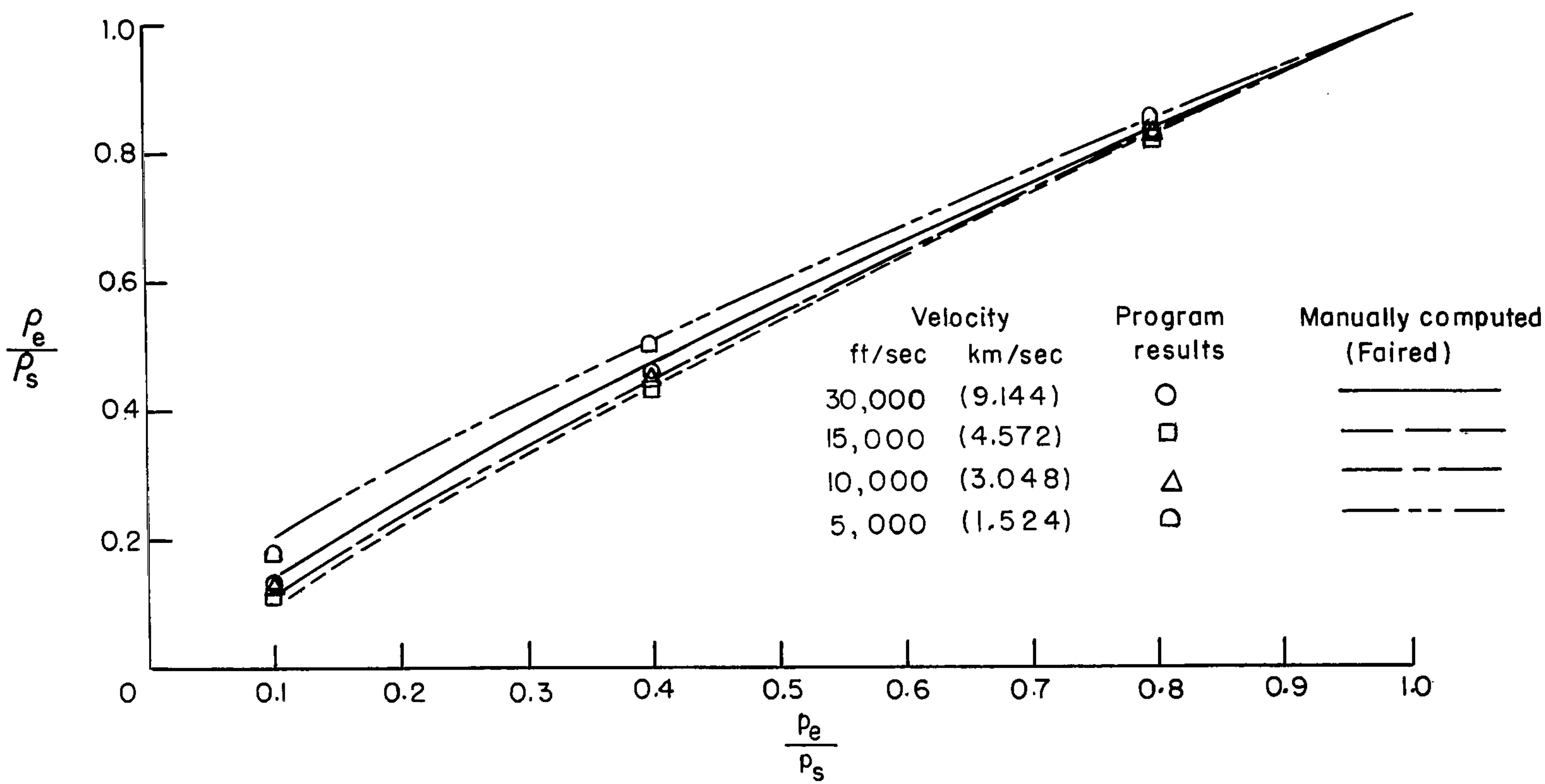


Figure 7.- Normalized density as a function of pressure for isentropic flow. Altitude, 150 000 feet (45.72 km).

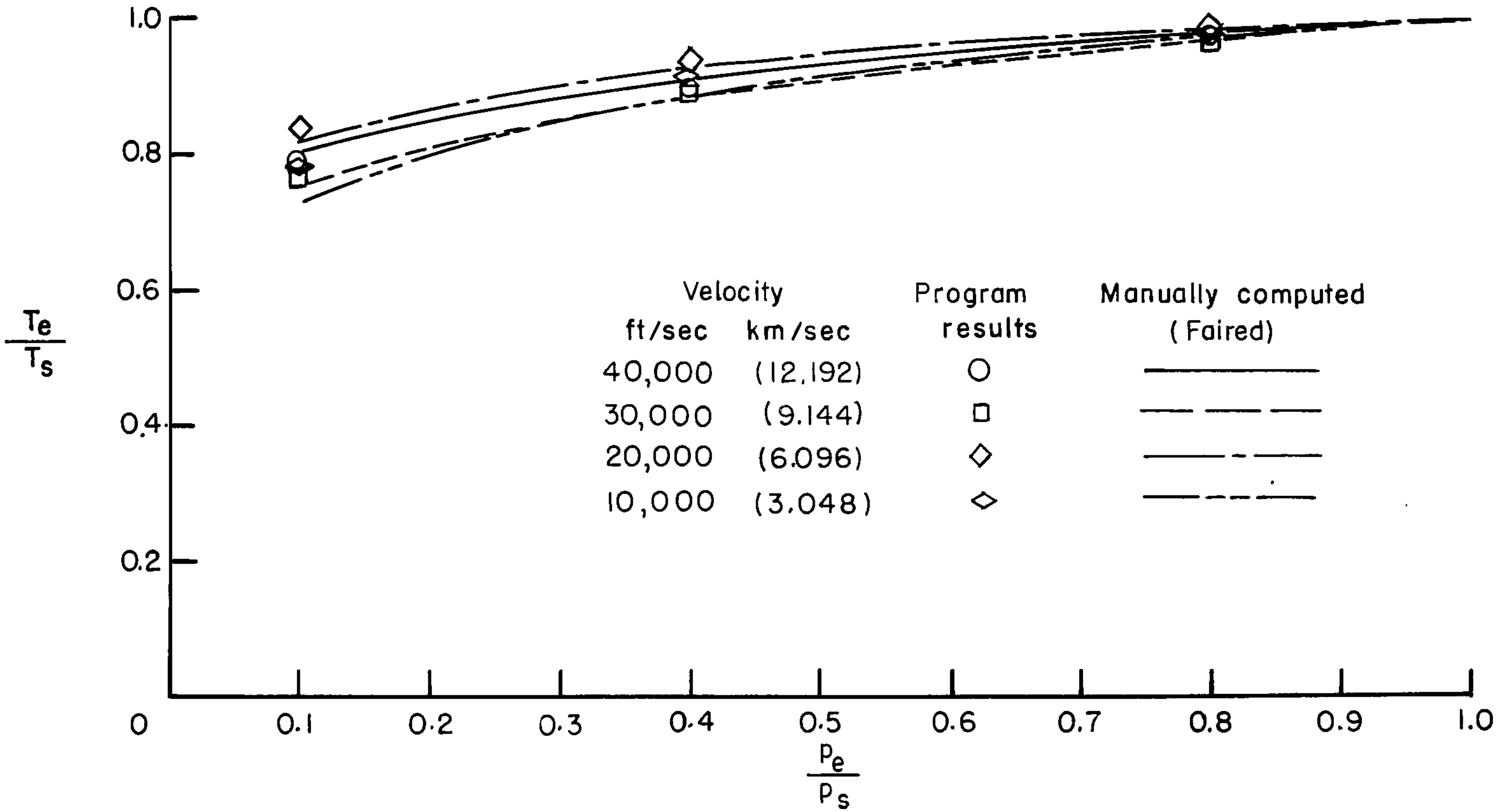


Figure 8.- Normalized temperature as a function of pressure for isentropic flow. Altitude, 150 000 feet (45.72 km).

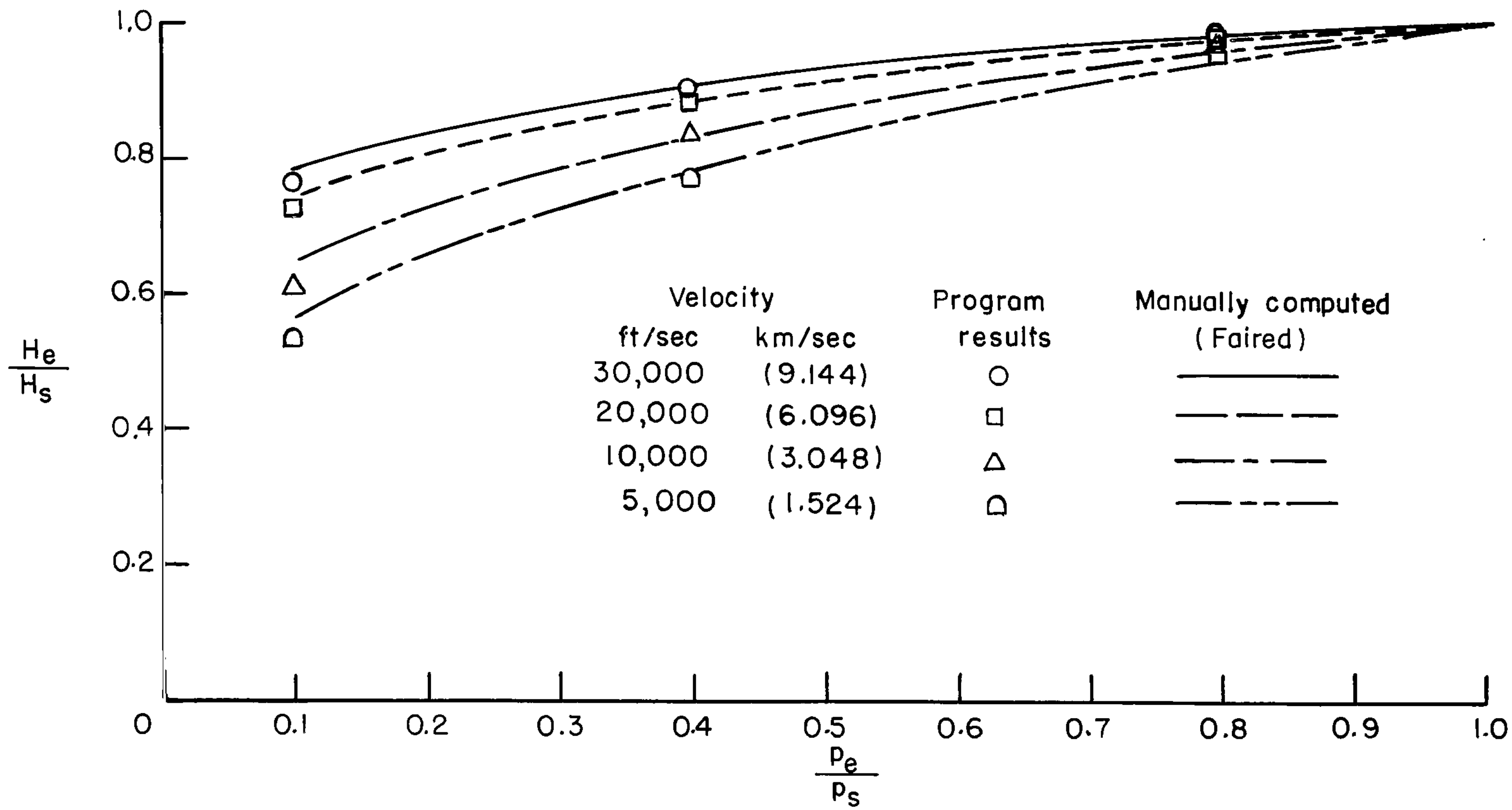


Figure 9.- Normalized enthalpy as a function of pressure for isentropic flow. Altitude, 150 000 feet (45.72 km).

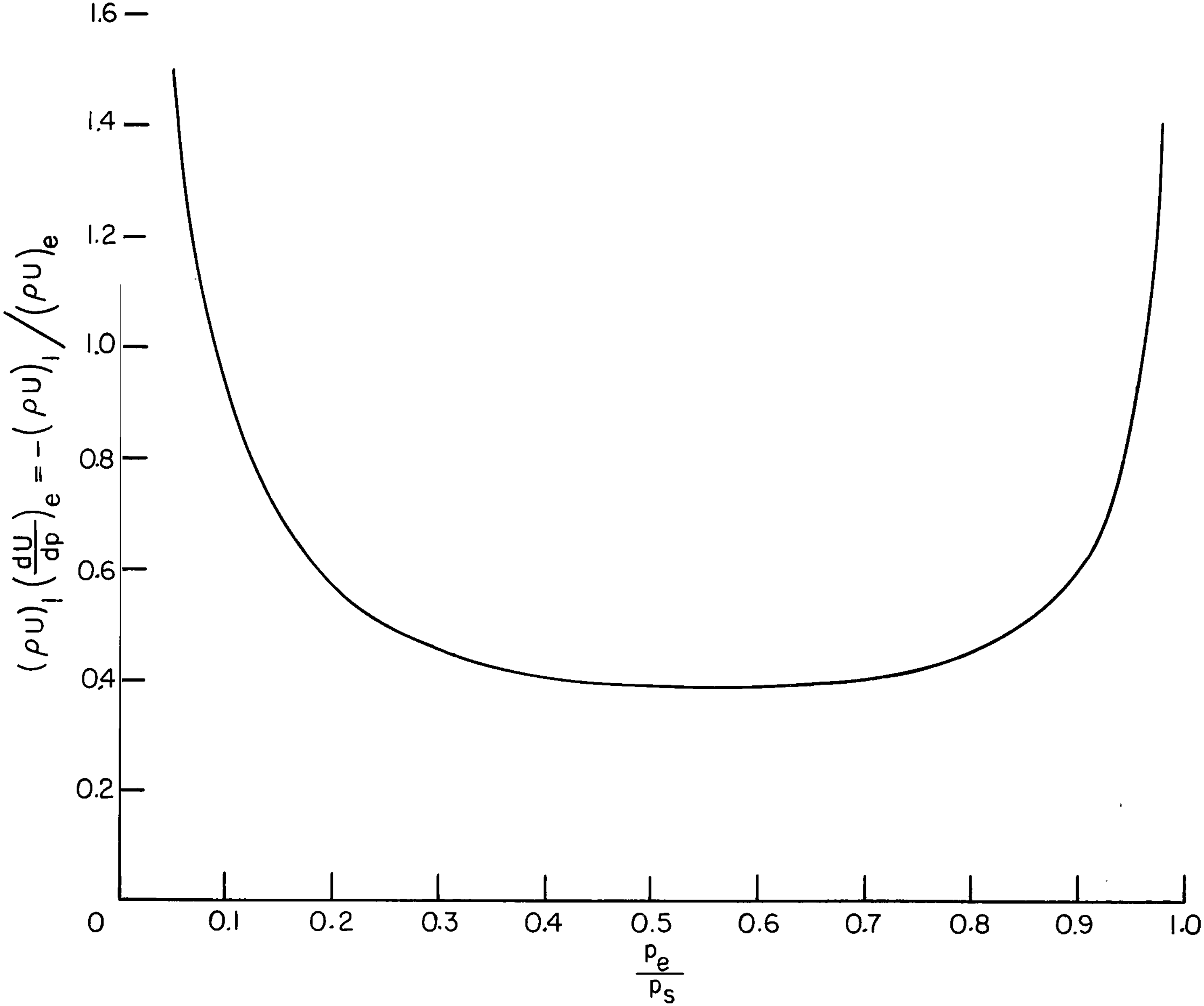


Figure 10.- Normalized derivative of velocity with pressure as a function of pressure for isentropic flow. Altitude, 150 000 feet (45.72 km); Velocity, 30 000 feet/sec (9.144 km/sec).

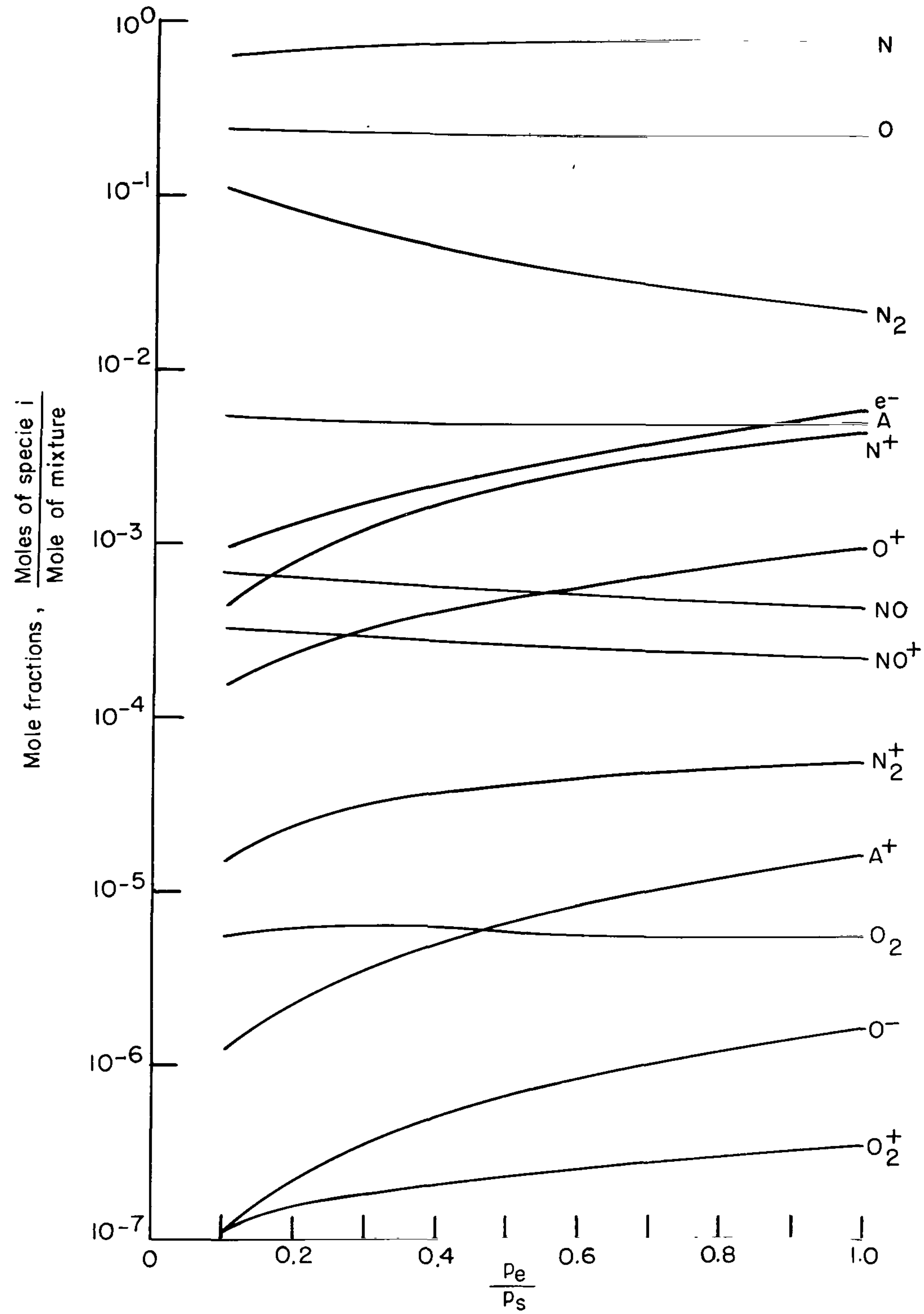


Figure 11.- Specie concentration in mole fractions as a function of pressure ratio for isentropic flow. Altitude, 150 000 feet (45.72 km); Velocity, 30 000 feet/sec (9.144 km/sec).

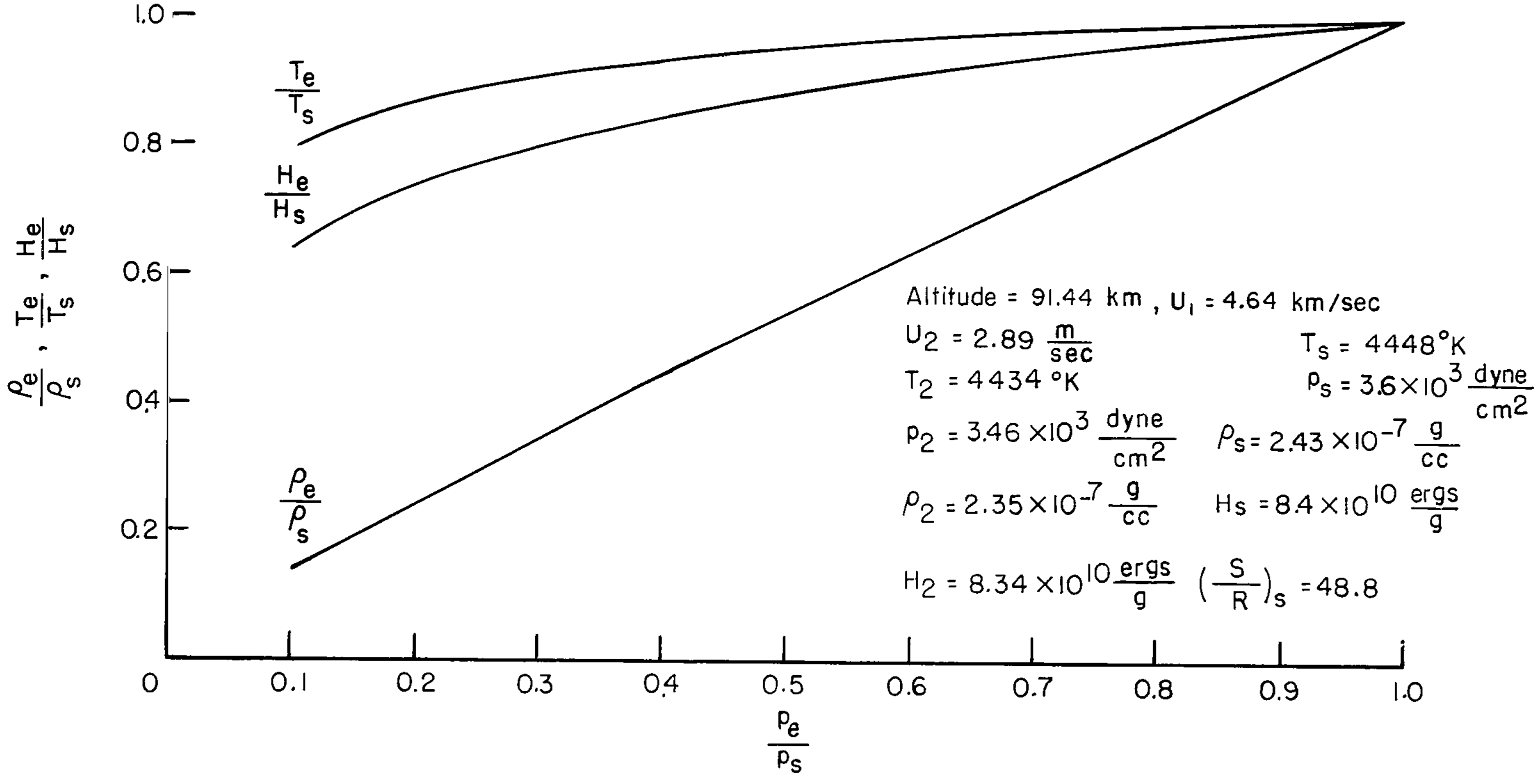


Figure 12.- Isentropic flow solutions in assumed Martian atmosphere for normalized density, temperature, and enthalpy as functions of pressure distribution.

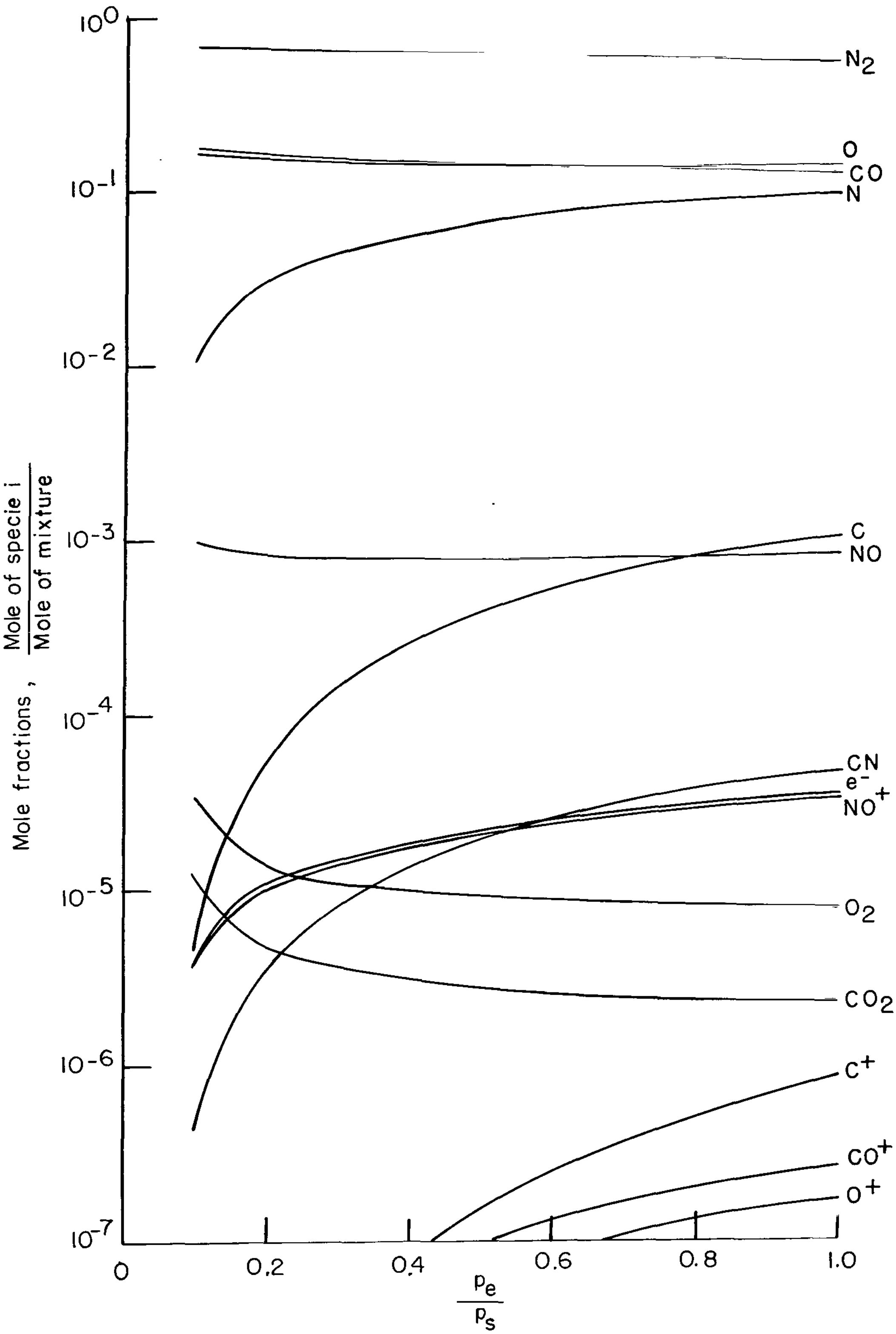


Figure 13.- Specie concentration in mole fraction based on isentropic flow and assumed Martian atmosphere as a function of pressure distribution. Altitude, 300 000 feet (91.44 km); Velocity, 15 200 feet/sec (4.64 km/sec).

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